Electronic Supplementary Information

A combined density functional theory and numerical simulation investigation of levels of chirality transfer and regioselectivity in the AIBN/$HSnBu_3$-mediated radical cyclizations of *N*-methyl-, *N*-ethyl- and *N*-isopropyl-substituted *ortho*-halo-*N*-acryloylanilides

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RSC New Journal of Chemistry

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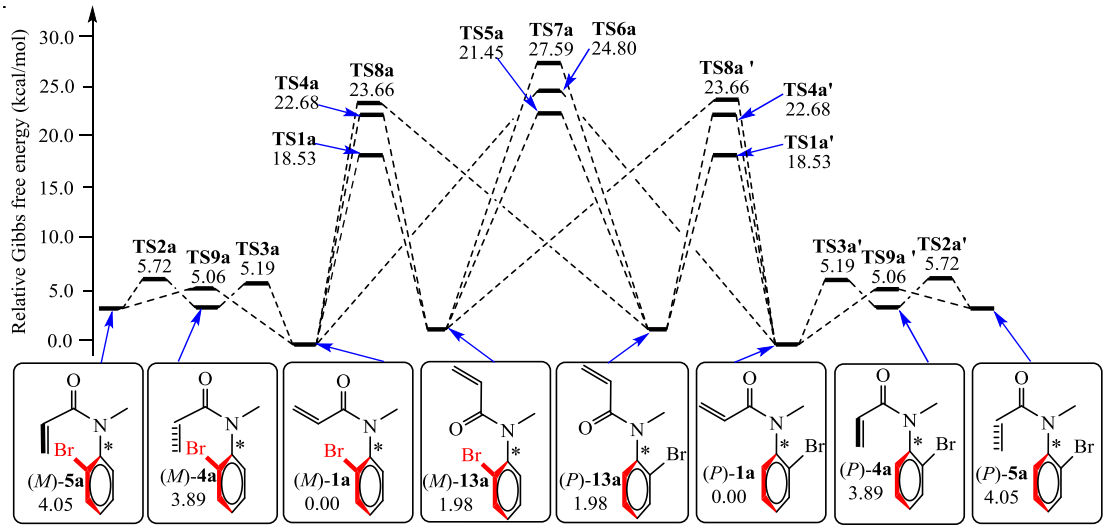


Figure S1 Computed isomerization profile for the conformational isomers of **1a**

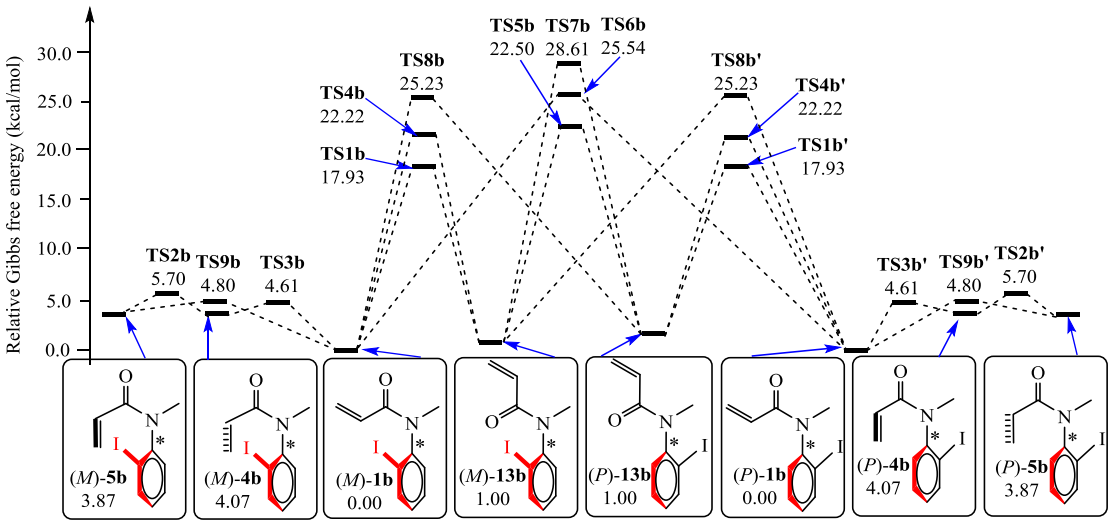


Figure S2 Computed isomerization profile for the conformational isomers of **1b**

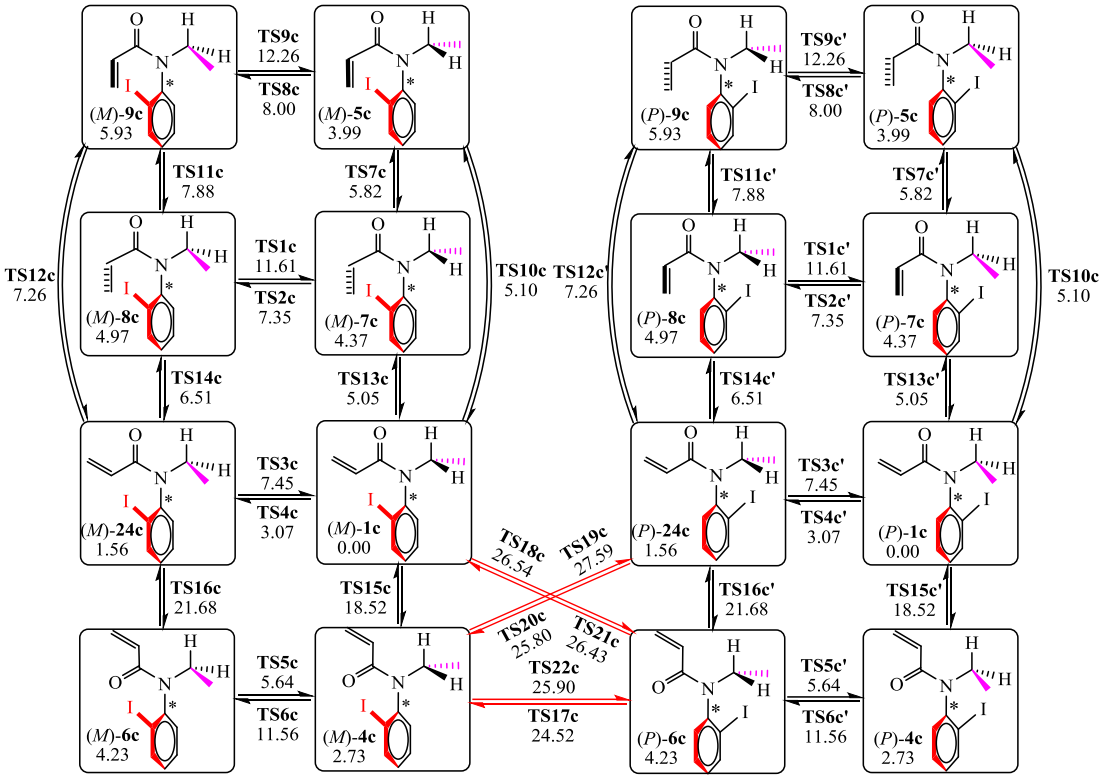


Figure S3 Computed isomerization profile for the conformational isomers of **1c**

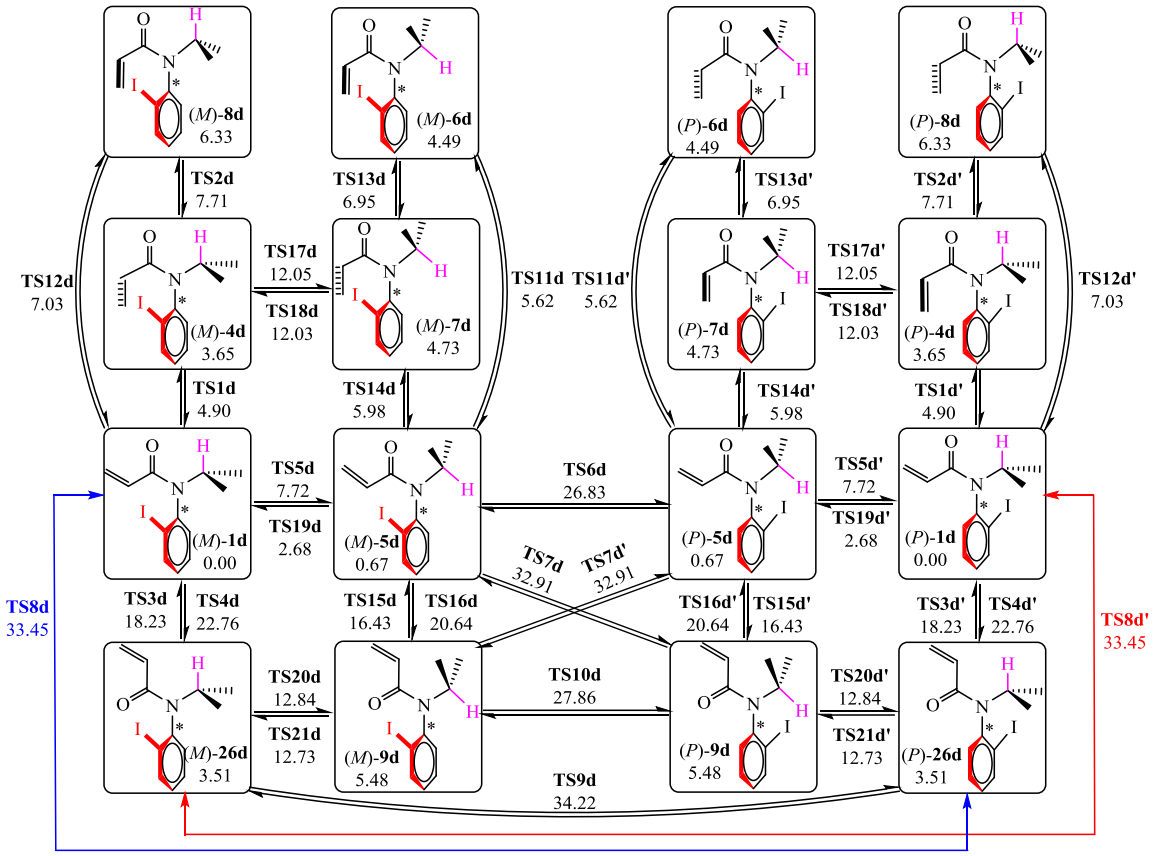
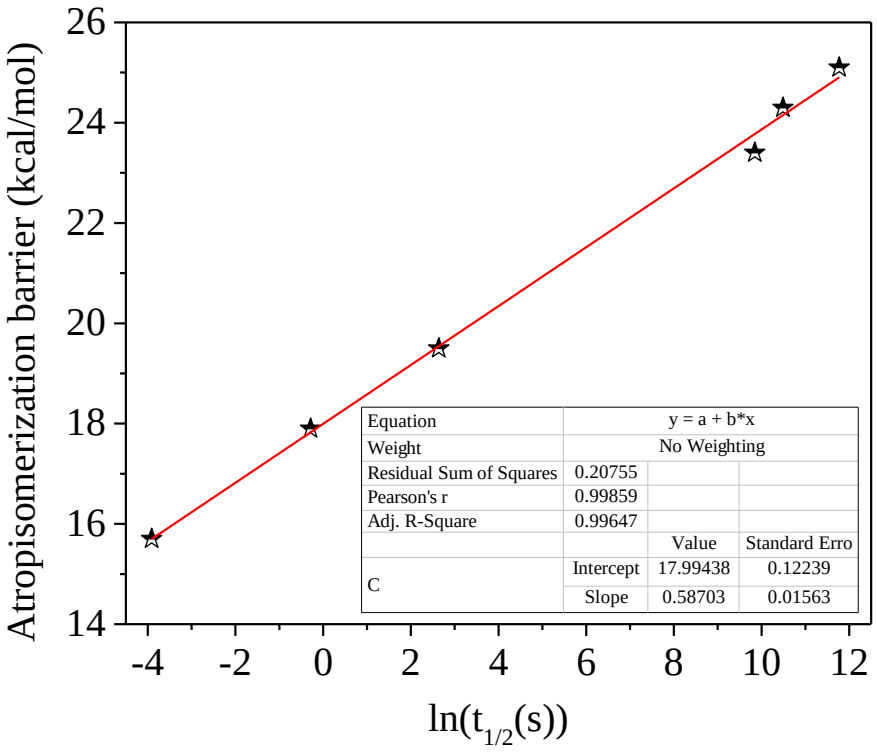
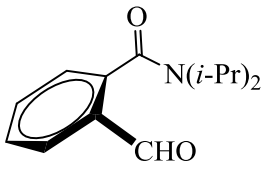


Figure S4 Computed isomerization profile of the conformational isomers of the substrate for system **D**. The energies used are the relative Gibbs free energies (in kcal/mol) with the lowest-lying (*M*)-**1d** as the zero reference point

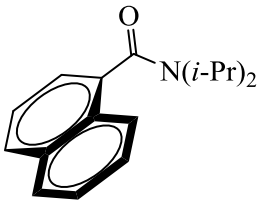




I1

$\Delta G^{\neq}_{rot}$ = 15.7 kcal/mol

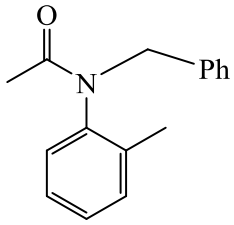
$t_{1/2}$ = 0.02 s at 298.15 K



I2

$\Delta G^{\neq}_{rot}$ = 17.9 kcal/mol

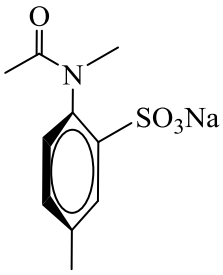
$t_{1/2}$ = 0.75 s at 298.15 K



I3

$\Delta G^{\neq}_{rot}$ = 19.3 kcal/mol

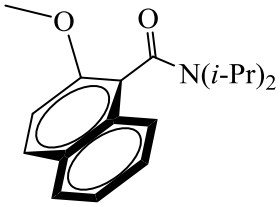
$t_{1/2}$ = 14 s at 298.15 K



I4

$\Delta G^{\neq}_{rot}$ = 23.4 kcal/mol

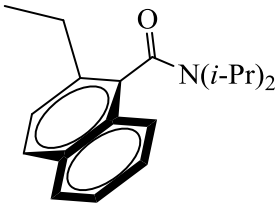
$t_{1/2}$ = 5.25 h at 298.15 K



I5

$\Delta G^{\neq}_{rot}$ = 24.3 kcal/mol

$t_{1/2}$ = 10 h at 298.15 K



I6

$\Delta G^{\neq}_{rot}$ = 25.1 kcal/mol

$t_{1/2}$ = 39 h at 298.15 K

Figure S5 Fitted relationship between the atropisomerization barriers and half-lives using the data of several experimentally available anilides at 298.15 K

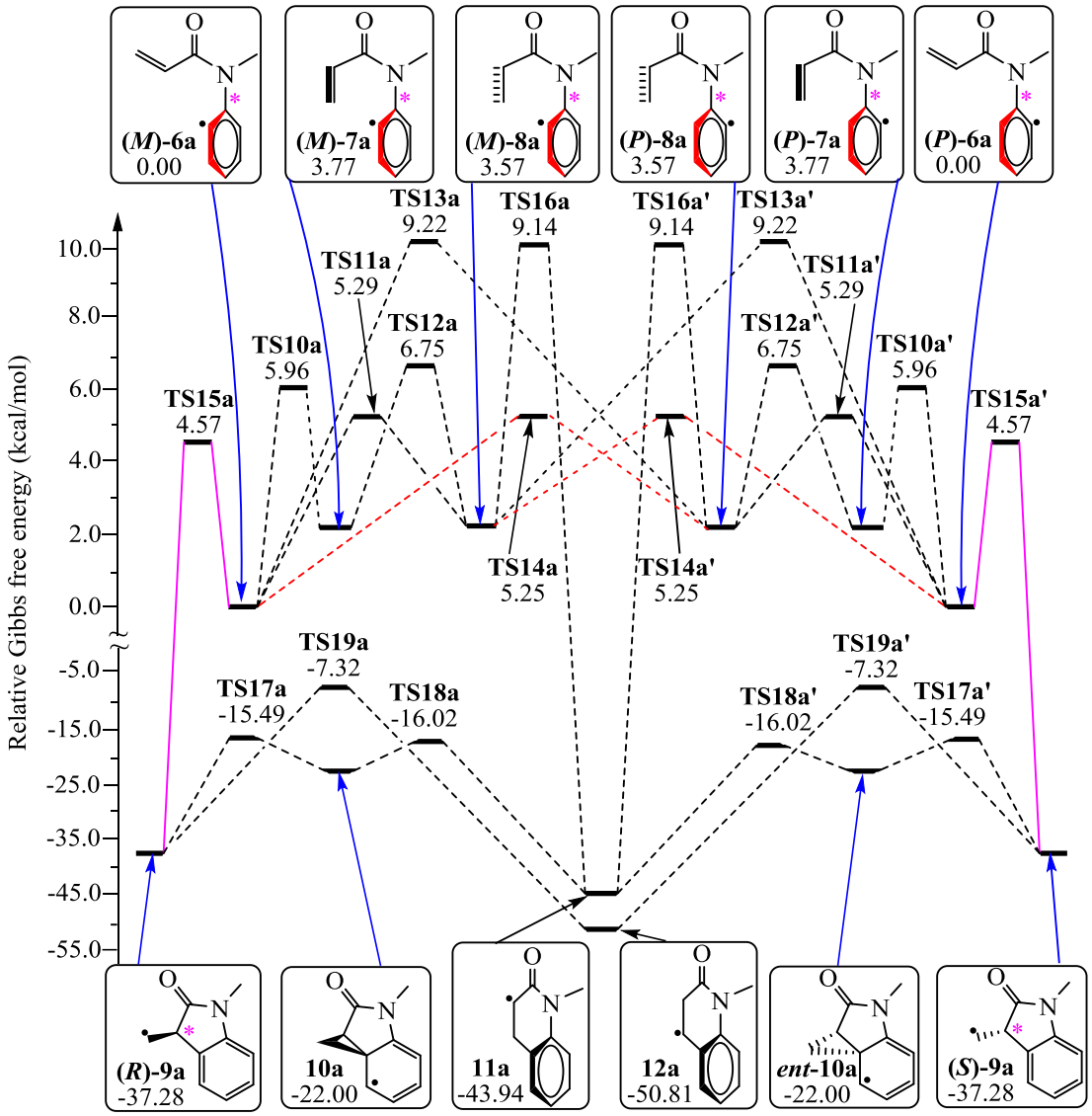


Figure S6 Computed radical isomerization and cyclization potential energy profile of the system **A** (383 K)

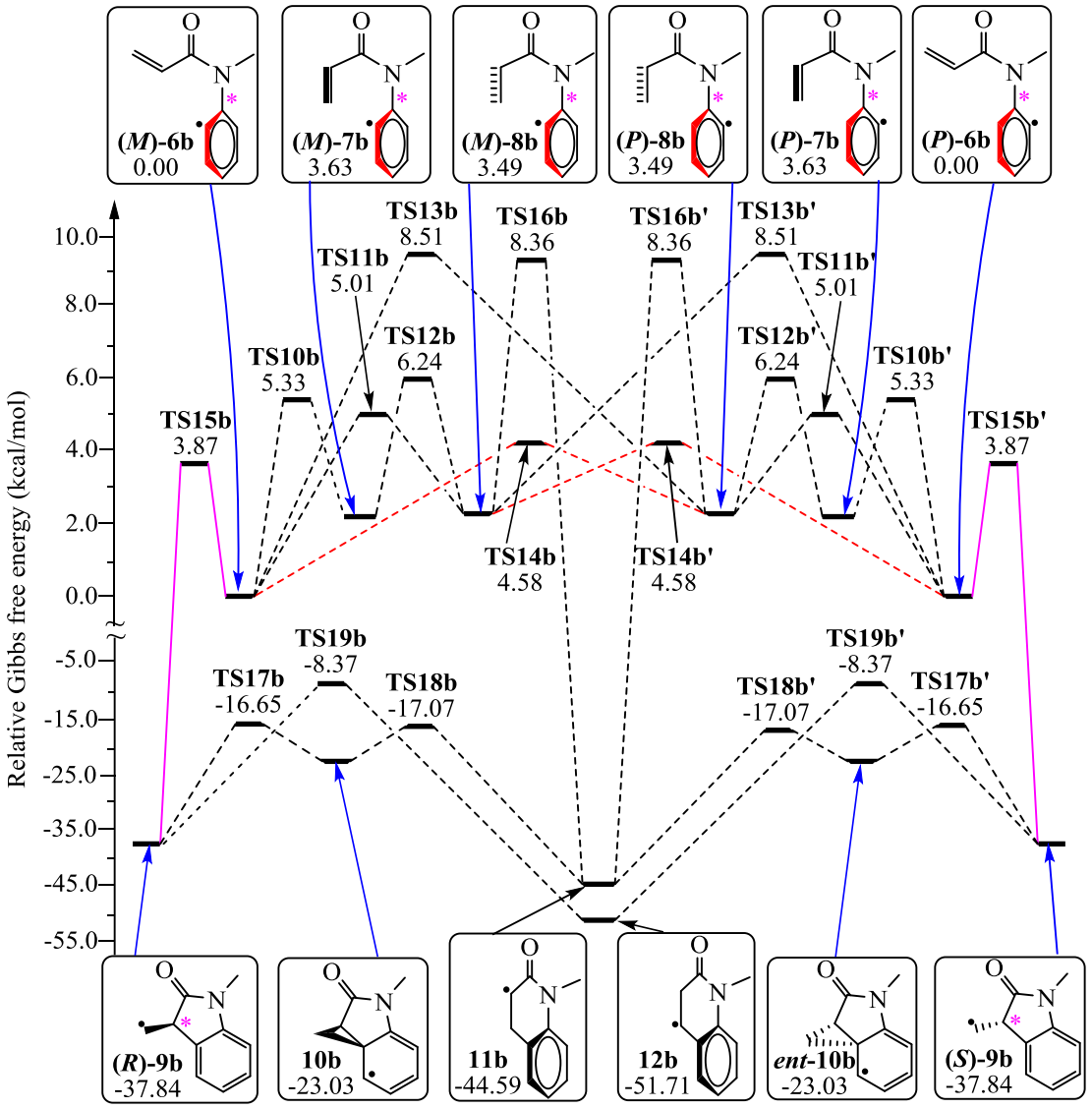


Figure S7 Computed radical isomerization and cyclization potential energy profile of the system **B** (298 K)

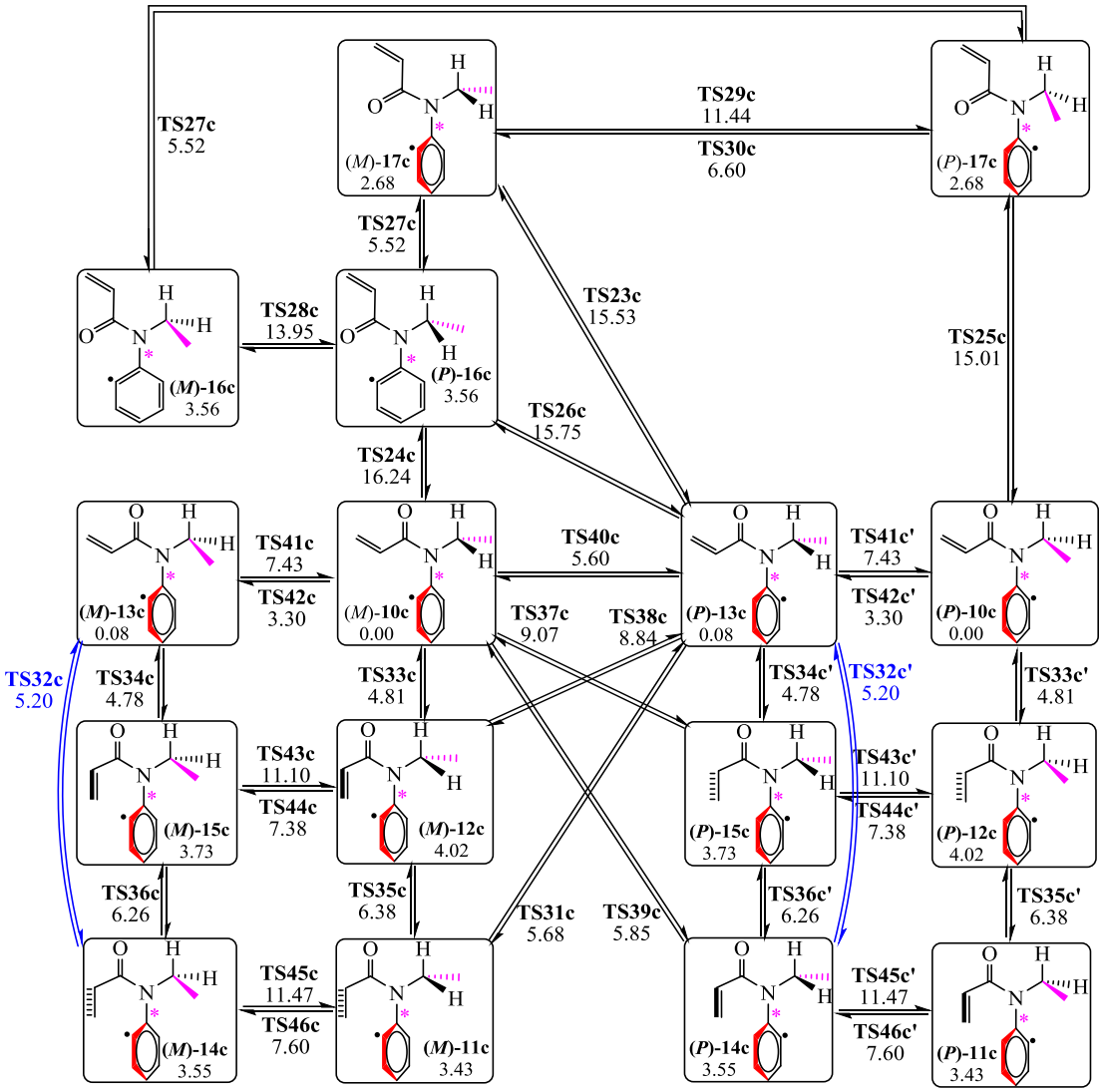


Figure S8 Computed radical isomerization potential energy profile of the system **C** (298 K)

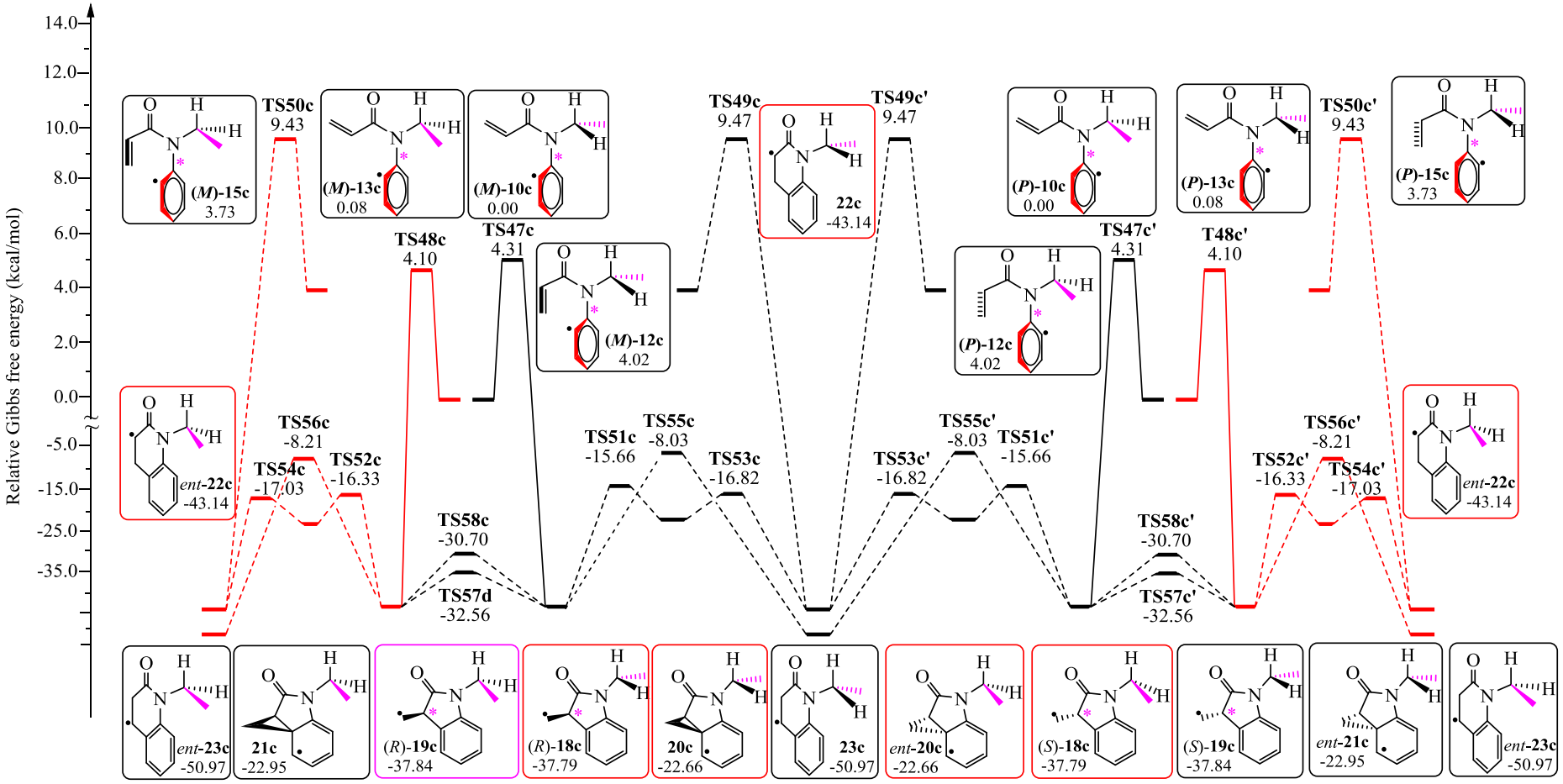


Figure S9 Computed competitive pathways between radical cyclization and neophyl-like rearrangement for the system **C** (298 K)

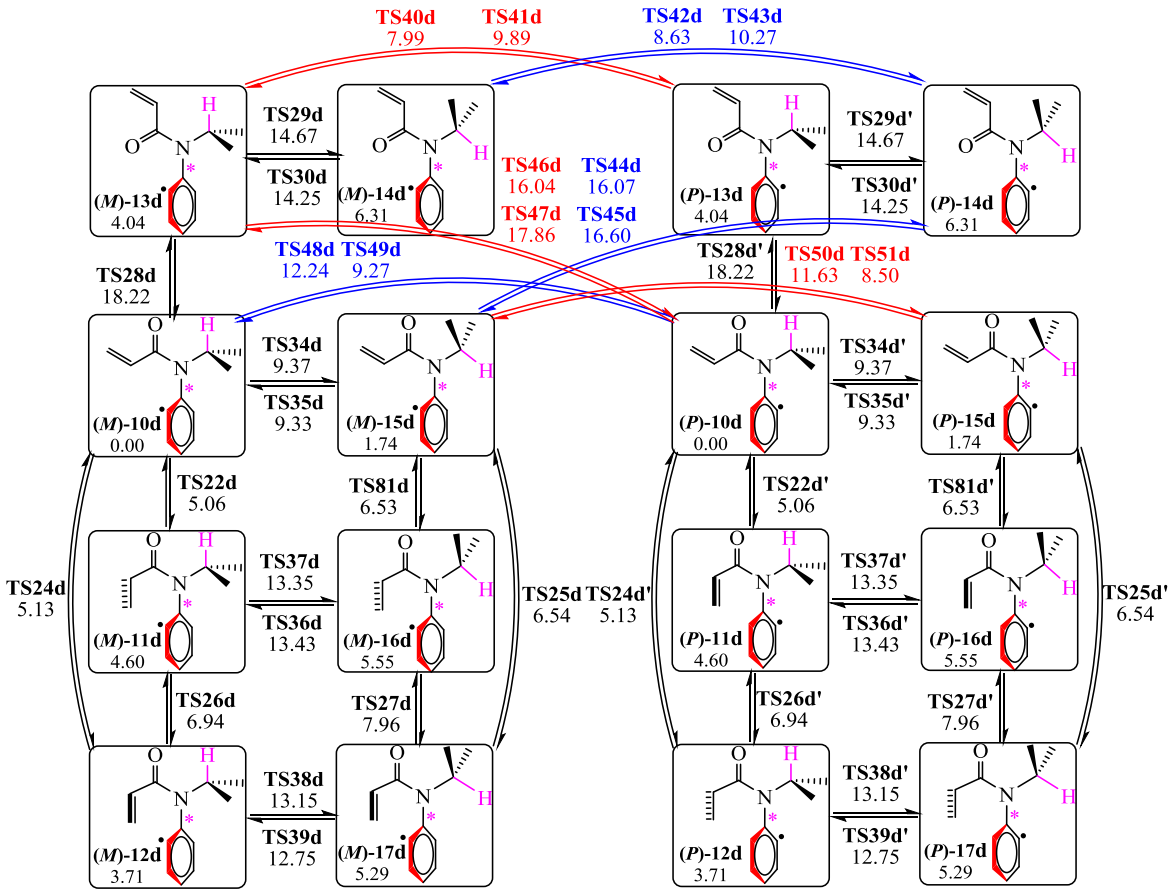


Figure S10 Computed isomerization potential energy profile of the radical reactants for system **D**. The energies used are the relative Gibbs free energies (in kcal/mol, 296 K) with the lowest-lying (*M*)-**10d** as the zero reference point

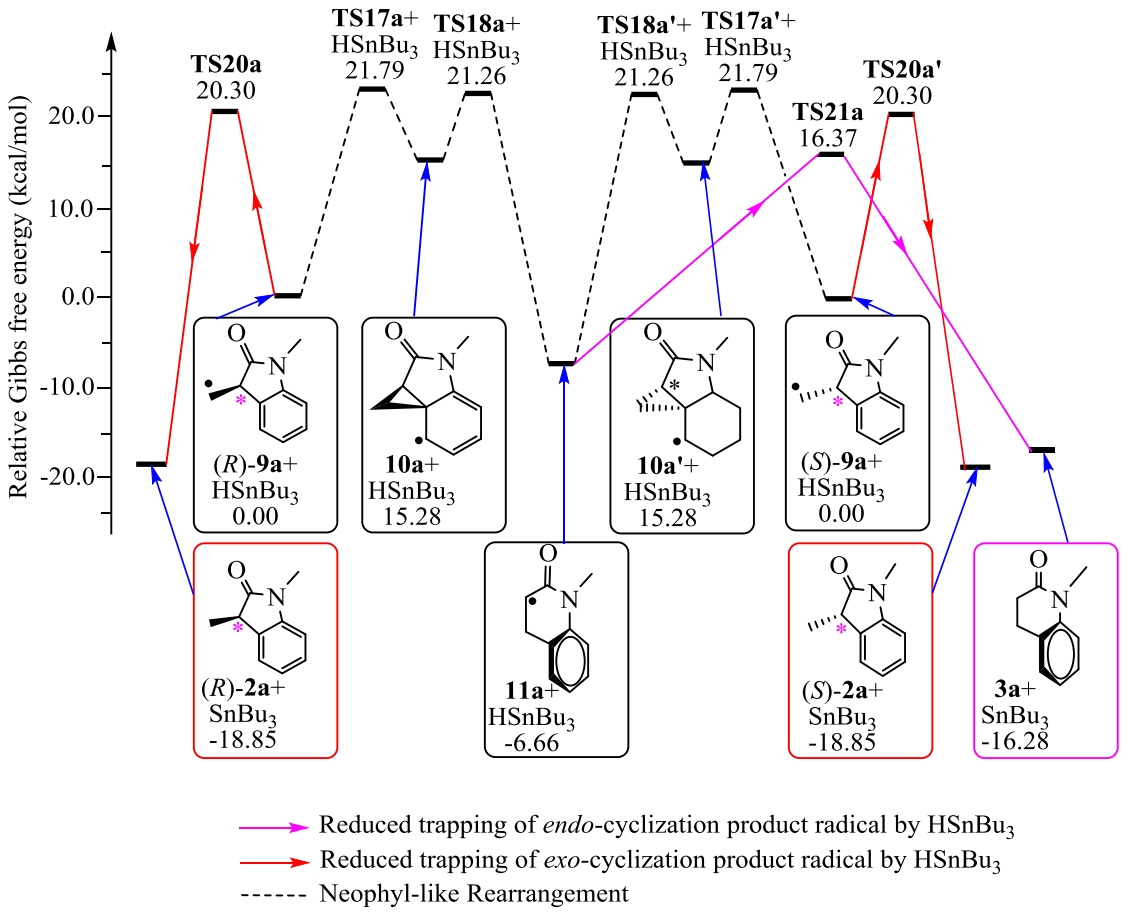


Figure S11 Computed competitive pathways between radical reduction and neophyl-like rearrangement for the system **A** (383 K)

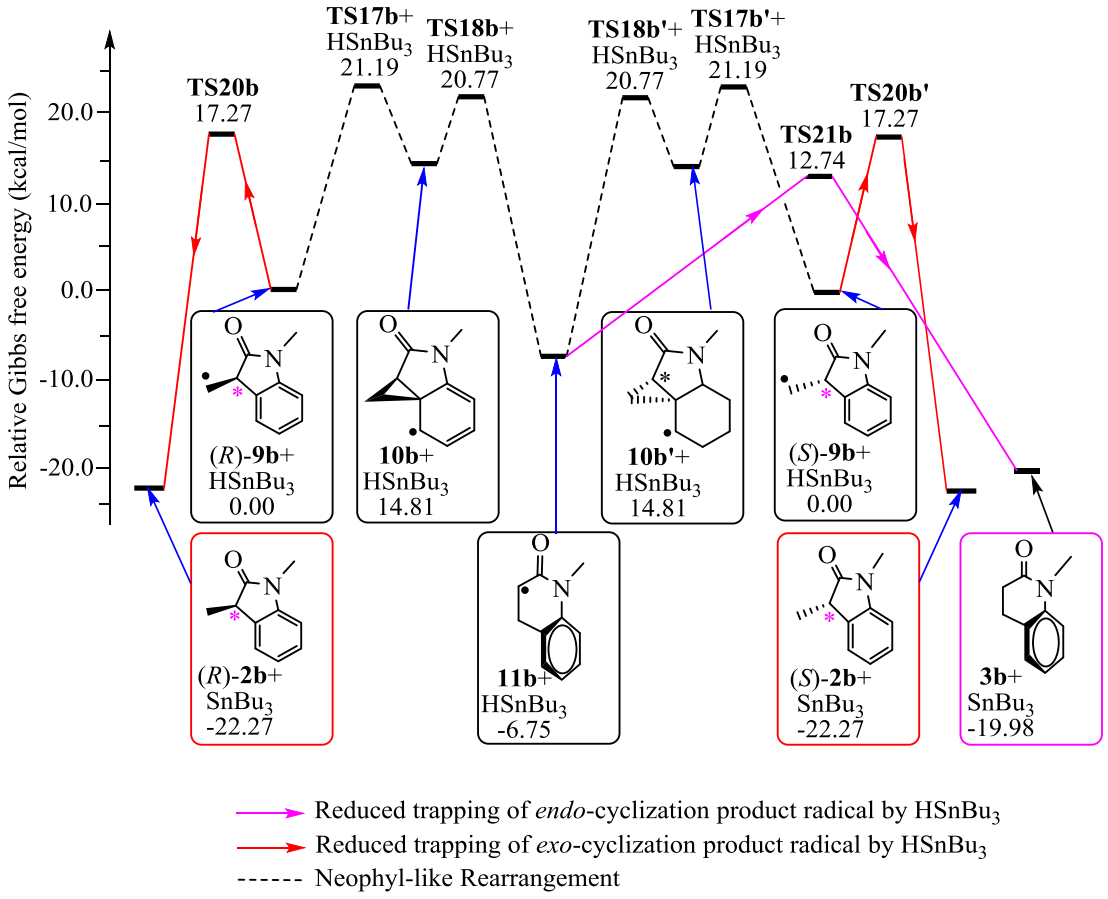


Figure S12 Computed competitive pathways between radical reduction and neophyl-like rearrangement for the system **B** (298 K)

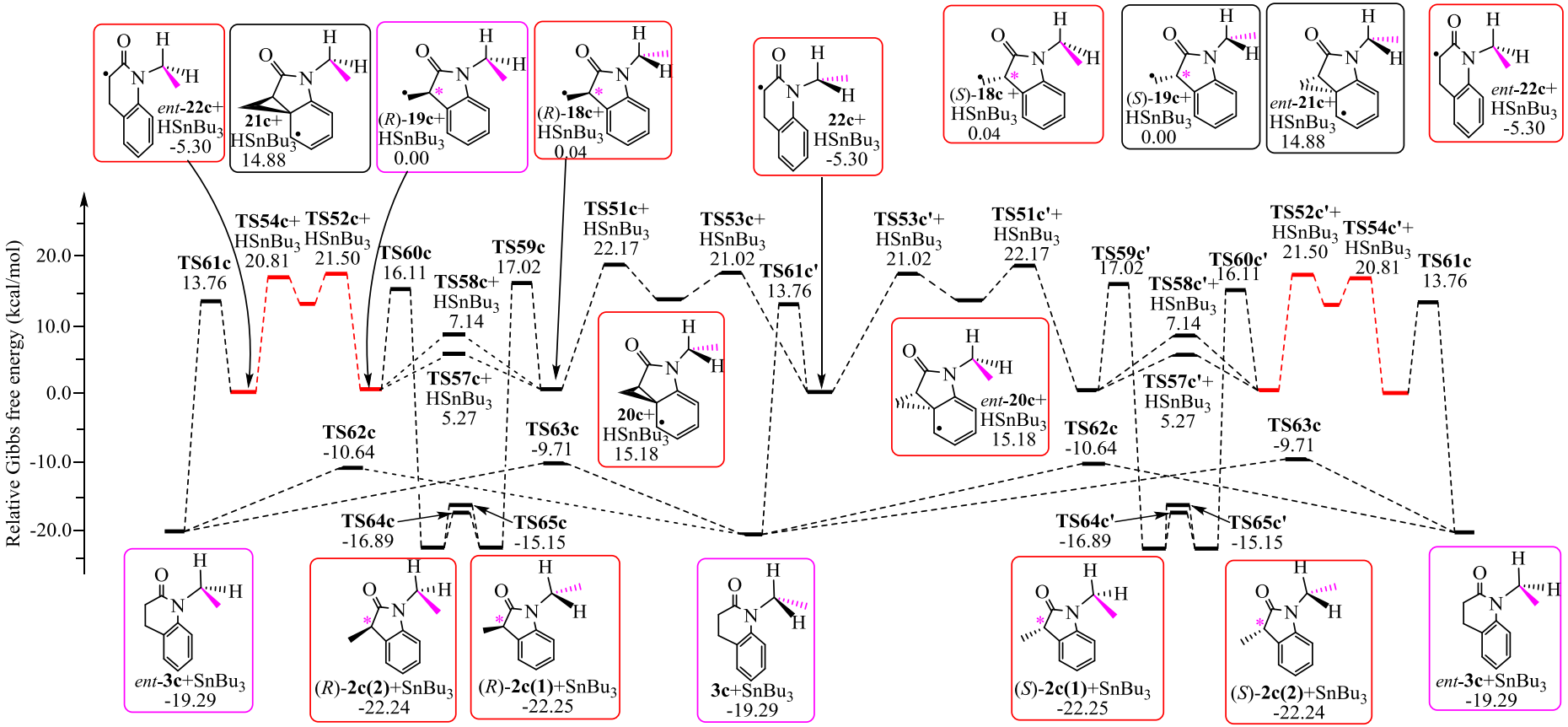


Figure S13 Computed competitive pathways between radical reduction and neophyl-like rearrangement for the system **C** (298 K)

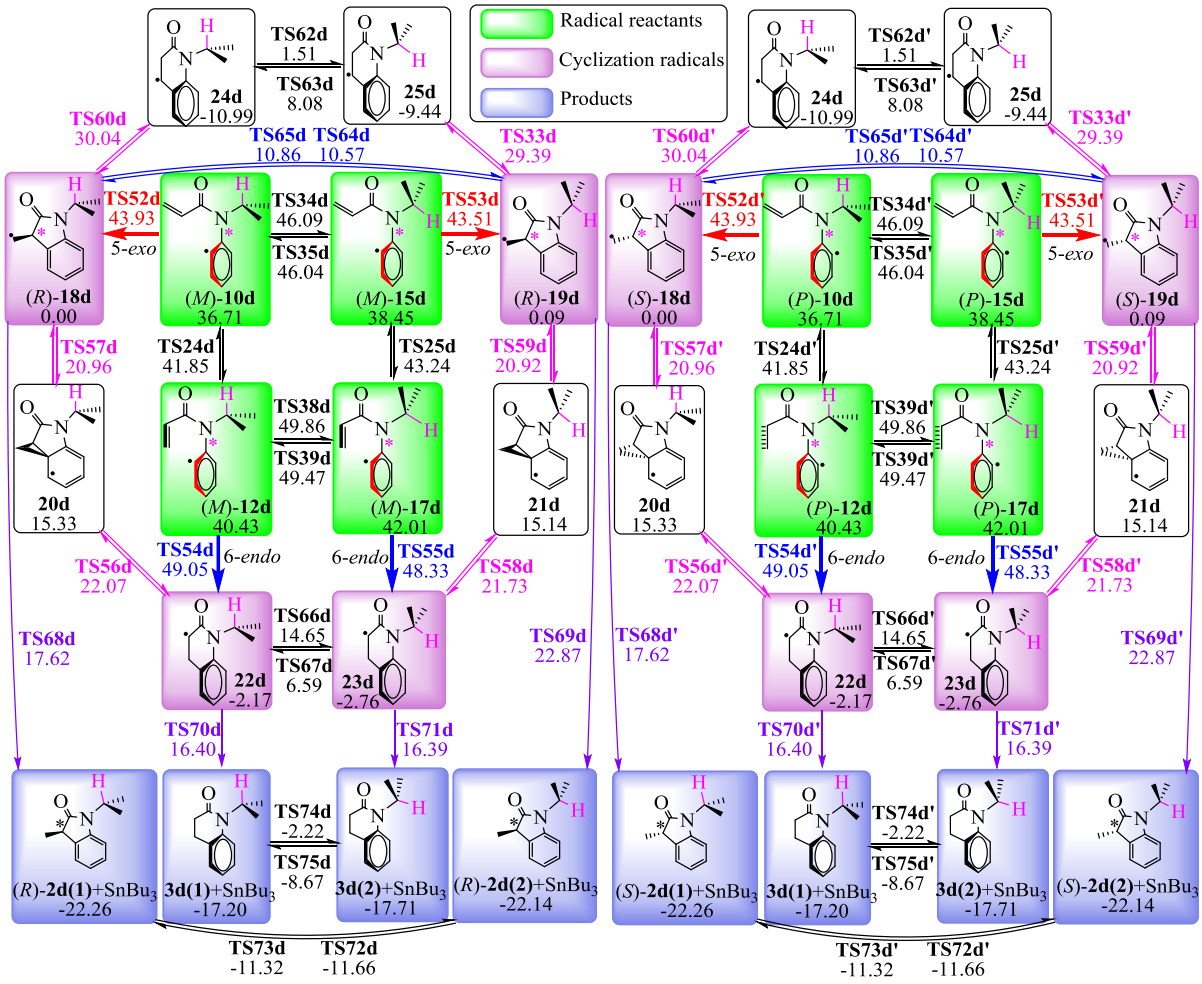


Figure S14 Radical cyclization and further reduction pathways of system **D**. The energies are relative Gibbs free energies (in kcal/mol, 296 K) with (*R*)-**18d** as the zero reference point

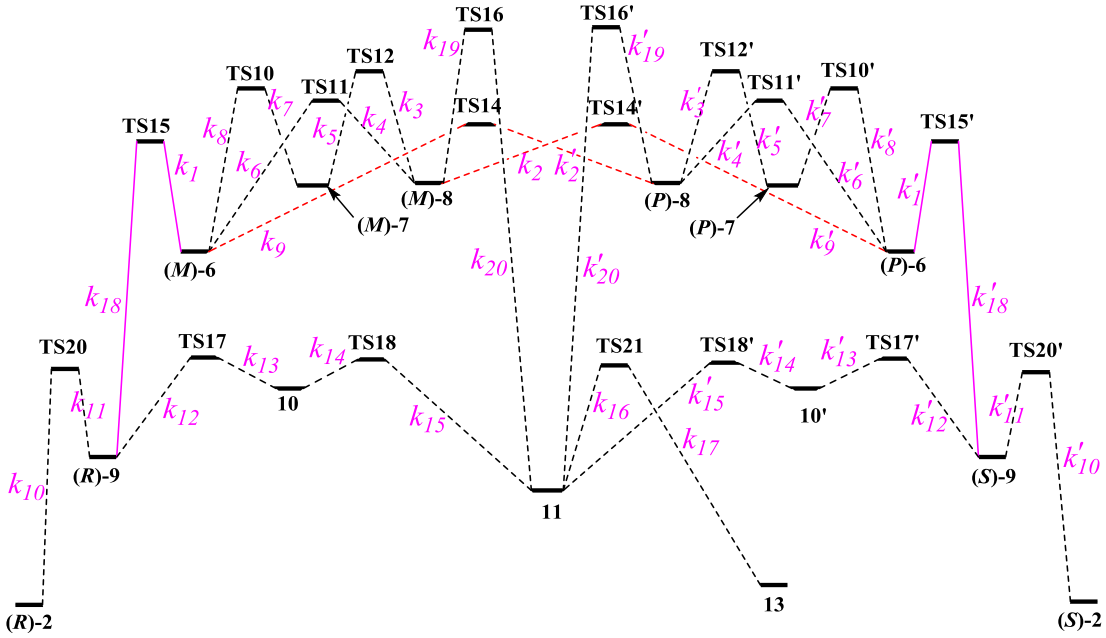


Figure S15 Schematic elementary reaction channels and names of the corresponding rate constants for the systems **A** and **B**

Table S1 Computed electronic total energies (E, in hartree), zero-point vibrational energies (ZPVE, in hartree/particle), enthalpies (H, in hartree, 383.15 K), Gibbs free energies (G, in hartree, 383.15 K), relative enthalpies (ΔH, in kcal/mol, 383.15 K), and relative Gibbs free energies (ΔG, in kcal/mol, 383.15 K) at the BH*and*HLYP/6-311++G(d,p)~SDD level of theory with $C_6H_5CH_3$ as the solvent for the isomers and their interconversion transition states of the substrate **1a**

Speaies	E	ZPVE	H	G	ΔH	ΔG
1a	-530.008042	0.183605	-529.987502	-530.065700	0.00	0.00
13a	-530.003655	0.183514	-529.983013	-530.062537	2.82	1.98
4a	-530.002187	0.183339	-529.981543	-530.059497	3.74	3.89
5a	-530.002759	0.183594	-529.982291	-530.059242	3.27	4.05
TS1a (**TS1a′**)	-529.980600	0.182778	-529.961065	-530.036174	16.59	18.53
TS2a (**TS2a′**)	-530.000274	0.183397	-529.980703	-530.056592	4.27	5.72
TS3a (**TS3a′**)	-530.001200	0.182767	-529.981429	-530.057422	3.81	5.19
TS4a (**TS4a′**)	-529.974685	0.182903	-529.955309	-530.029559	20.20	22.68
TS5a	-529.977916	0.184513	-529.959046	-530.031512	17.86	21.45
TS6a	-529.972864	0.184377	-529.954005	-530.026173	21.02	24.80
TS7a	-529.967045	0.183781	-529.947975	-530.021734	24.80	27.59
TS8a (**TS8a′**)	-529.974004	0.183170	-529.954680	-530.027994	20.60	23.66
TS9a (**TS9a′**)	-530.001369	0.182778	-529.981594	-530.057629	3.71	5.06

Table S2 Computed electronic total energies (E, in hartree), zero-point vibrational energies (ZPVE, in hartree/particle), enthalpies (H, in hartree, 298.15 K), Gibbs free energies (G, in hartree, 298.15 K), relative enthalpies (ΔH, in kcal/mol, 298.15 K), and relative Gibbs free energies (ΔG, in kcal/mol, 298.15 K) at the BH*and*HLYP/6-311++G(d,p)~SDD level of theory with $C_6H_5CH_3$ as the solvent for the isomers and their interconversion transition states of the substrate **1b**

Species	E	ZPVE	H	G	ΔH	ΔG
1b	-528.040325	0.183289	-528.026718	-528.082130	0.00	0.00
13b	-528.035806	0.183083	-528.021996	-528.080534	2.96	1.00
4b	-528.033915	0.182961	-528.020185	-528.075652	4.10	4.07
5b	-528.034719	0.183180	-528.021128	-528.075955	3.51	3.87
TS1b (**TS1b′**)	-528.012947	0.182441	-528.000096	-528.053560	16.71	17.93
TS2b (**TS2b′**)	-528.032552	0.183203	-528.019712	-528.073039	4.40	5.70
TS3b (**TS3b′**)	-528.033191	0.182344	-528.020059	-528.074776	4.18	4.61
TS4b (**TS4b′**)	-528.006788	0.182504	-527.994057	-528.046726	20.50	22.22
TS5b	-528.007111	0.184177	-527.994845	-528.046272	20.00	22.50
TS6b	-528.002542	0.184066	-527.990307	-528.041425	22.85	25.54
TS7b	-527.996943	0.183734	-527.984583	-528.036540	26.44	28.61
TS8b (**TS8b′**)	-528.002582	0.182868	-527.989932	-528.041925	23.08	25.23
TS9b (**TS9b′**)	-528.033409	0.182417	-528.020303	-528.074486	4.03	4.80

Table S3 Computed electronic total energies (E, in hartree), zero-point vibrational energies (ZPVE, in hartree/particle), enthalpies (H, in hartree, 298.15 K), Gibbs free energies (G, in hartree, 298.15 K), relative enthalpies (ΔH, in kcal/mol, 298.15 K), and relative Gibbs free energies (ΔG, in kcal/mol, 298.15 K) at the BH*and*HLYP/6-311++G(d,p)~SDD level of theory with $C_6H_5CH_3$ as the solvent for the isomers and their interconversion transition states of the substrate **1c**

Species	E	ZPVE	H	G	ΔH	ΔG
1c	-567.310476	0.212793	-567.295754	-567.353612	0.00	0.00
3c	-567.308167	0.212829	-567.293474	-567.351127	1.43	1.56
4c	-567.305901	0.212711	-567.291121	-567.349255	2.91	2.73
5c	-567.304587	0.212598	-567.289841	-567.347246	3.71	3.99
6c	-567.304045	0.212851	-567.289365	-567.346877	4.01	4.23
7c	-567.303658	0.212530	-567.288853	-567.346647	4.33	4.37
8c	-567.303096	0.212589	-567.288368	-567.345693	4.63	4.97
9c	-567.302011	0.212602	-567.287323	-567.344163	5.29	5.93
TS1c (**TS1c′**)	-567.293475	0.212336	-567.279485	-567.335109	10.21	11.61
TS2c (**TS2c′**)	-567.300452	0.212423	-567.286486	-567.341892	5.82	7.35
TS3c (**TS3c′**)	-567.299881	0.212641	-567.285956	-567.341745	6.15	7.45
TS4c (**TS4c′**)	-567.307066	0.212625	-567.293139	-567.348727	1.64	3.07
TS5c (**TS5c′**)	-567.302078	0.212459	-567.287959	-567.344629	4.89	5.64
TS6c (**TS6c′**)	-567.293297	0.212826	-567.279389	-567.335194	10.27	11.56
TS7c (**TS7c′**)	-567.302571	0.212664	-567.288617	-567.344335	4.48	5.82
TS8c (**TS8c′**)	-567.299054	0.212492	-567.285120	-567.340860	6.67	8.00
TS9c (**TS9c′**)	-567.292577	0.212483	-567.278624	-567.334078	10.75	12.26
TS10c (**TS10c′**)	-567.303582	0.212080	-567.289464	-567.345485	3.95	5.10
TS11c (**TS11c′**)	-567.299706	0.212753	-567.285815	-567.341049	6.24	7.88
TS12c (**TS12c′**)	-567.300286	0.211978	-567.286141	-567.342048	6.03	7.26
TS13c (**TS13c′**)	-567.303239	0.211939	-567.289053	-567.345565	4.20	5.05
TS14c (**TS14c′**)	-567.301327	0.212131	-567.28725	-567.343241	5.34	6.51
TS15c (**TS15c′**)	-567.281972	0.211625	-567.267829	-567.324099	17.52	18.52
TS16c (**TS16c′**)	-567.276955	0.211630	-567.262834	-567.319066	20.66	21.68
TS17c	-567.273819	0.213167	-567.260213	-567.314536	22.30	24.52
TS18c	-567.270266	0.212012	-567.256295	-567.311325	24.76	26.54
TS19c	-567.268718	0.212831	-567.255001	-567.309648	25.57	27.59
TS20c	-567.271491	0.212010	-567.257531	-567.312496	23.99	25.80
TS21c	-567.270050	0.212092	-567.256125	-567.311495	24.87	26.43
TS22c	-567.271671	0.213888	-567.258242	-567.312340	23.54	25.90

Table S4 Computed electronic total energies (E, in hartree), zero-point vibrational energies (ZPVE, in hartree/particle), enthalpies (H, in hartree, 296.15 K), Gibbs free energies (G, in hartree, 296.15 K), relative enthalpies (ΔH, in kcal/mol, 296.15 K), and relative Gibbs free energies (ΔG, in kcal/mol, 296.15 K) at the BH*and*HLYP/6-311++G(d,p)~SDD level of theory with C_6H_6 as the solvent for the isomers and their interconversion transition states of the substrate **1d**

Species	E	ZPVE	H	G	ΔH	ΔG
1d	-606.576908	0.241618	-606.560951	-606.620816	0.00	0.00
26d	-606.571419	0.241726	-606.555481	-606.615225	3.43	3.51
4d	-606.571117	0.241307	-606.555076	-606.615002	3.69	3.65
5d	-606.575592	0.241390	-606.559535	-606.619753	0.89	0.67
6d	-606.570212	0.241337	-606.554190	-606.613663	4.24	4.49
7d	-606.569237	0.241086	-606.553084	-606.613275	4.94	4.73
8d	-606.567516	0.241472	-606.551616	-606.610731	5.86	6.33
9d	-606.567649	0.241538	-606.551536	-606.612091	5.91	5.48
TS1d (**TS1d′**)	-606.570171	0.240842	-606.554813	-606.613004	3.85	4.90
TS2d (**TS2d′**)	-606.565298	0.241701	-606.550207	-606.608530	6.74	7.71
TS3d (**TS3d′**)	-606.548673	0.240523	-606.533330	-606.591767	17.33	18.23
TS4d (**TS4d′**)	-606.541051	0.240355	-606.525606	-606.584547	22.18	22.76
TS5d (**TS5d′**)	-606.565343	0.241511	-606.550252	-606.608534	6.71	7.71
TS6d	-606.535972	0.241217	-606.520881	-606.578065	25.14	26.83
TS7d (**TS7d′**)	-606.525446	0.241151	-606.510173	-606.568375	31.86	32.91
TS8d (**TS8d′**)	-606.524837	0.240768	-606.509402	-606.567512	32.35	33.45
TS9d	-606.523889	0.241659	-606.508706	-606.566279	32.78	34.22
TS10d	-606.534223	0.241486	-606.519089	-606.576419	26.27	27.86
TS11d (**TS11d′**)	-606.568634	0.240650	-606.553155	-606.611865	4.89	5.62
TS12d (**TS12d′**)	-606.566849	0.240888	-606.551541	-606.609613	5.90	7.03
TS13d (**TS13d′**)	-606.566840	0.241330	-606.551555	-606.609747	5.90	6.95
TS14d (**TS14d′**)	-606.568050	0.240641	-606.552536	-606.611282	5.28	5.98
TS15d (**TS15d′**)	-606.551471	0.240481	-606.536081	-606.594636	15.61	16.43
TS16d (**TS16d′**)	-606.543464	0.239895	-606.527820	-606.587931	20.79	20.64
TS17d (**TS17d′**)	-606.559104	0.241238	-606.543988	-606.601614	10.64	12.05
TS18d (**TS18d′**)	-606.559018	0.241222	-606.543894	-606.601647	10.70	12.03
TS19d (**TS19d′**)	-606.573881	0.241540	-606.558811	-606.616266	1.34	2.86
TS20d (**TS20d′**)	-606.557478	0.241620	-606.542396	-606.600354	11.64	12.84
TS21d (**TS21d′**)	-606.557813	0.241566	-606.542749	-606.600522	11.42	12.73

Table S5 Computed electronic total energies with zero-point energy correction (E+ZPVE, in hartree), enthalpies, (H, in hartree), and Gibbs free energies (G, in hartree) for the stationary points **1a** and **TS5a** at different levels of theory

Levels of theory	E+ZPVE		H		G	
	1a	**TS5a**	**1a**	**TS5a**	**1a**	**TS5a**
BH*and*HLYP/6-31+G(d)	-3088.244960	-3088.212376	-3088.231683	-3088.200565	-3088.285746	-3088.250294
BH*and*HLYP/6-311++G(d,p)	-3090.789226	-3090.759175	-3090.775762	-3090.747080	-3090.830410	-3090.797523
BH*and*HLYP/aug-*cc*-pVDZ	-3090.733007	-3090.703468	-3090.719536	-3090.691360	-3090.774206	-3090.741832
B3LYP/6-31+G(d)	-3088.622740	-3088.592751	-3088.609165	-3088.580567	-3088.663714	-3088.630994
B3LYP/6-311++G(d,p)	-3091.157426	-3091.129646	-3091.143601	-3091.117135	-3091.198950	-3091.168412
B3LYP/aug-*cc*-pVDZ	-3091.089525	-3091.062498	-3091.075718	-3091.050001	-3091.130888	-3091.101211
M052X/6-31+G(d)	-3088.539516	-3088.506481	-3088.526767	-3088.494432	-3088.579425	-3088.544617
M052X/6-311++G(d,p)	-3091.025042	-3090.995782	-3091.011487	-3090.983462	-3091.066077	-3091.034395
M052X/aug-*cc*-pVDZ	-3090.971329	-3090.942763	-3090.957757	-3090.930435	-3091.012429	-3090.981416

Table S6 Computed electronic total energies with zero-point energy correction (E+ZPVE, in hartree), enthalpies, (H, in hartree), and Gibbs free energies (G, in hartree) for the stationary points **1b** and **TS5b** at different levels of theory

Levels of theory	E+ZPVE		H		G	
	1b	**TS5b**	**1b**	**TS5b**	**1b**	**TS5b**
BH*and*HLYP/6-31+G(d)~SDD	-527.918971	-527.885112	-527.905405	-527.872899	-527.960703	-527.924196
BH*and*HLYP/6-311++G(d,p)~SDD	-528.040109	-528.006938	-528.026503	-527.994673	-528.081911	-528.046100
BH*and*HLYP/6-31+G(d)~LANL2DZ	-527.894747	-527.860514	-527.881198	-527.848307	-527.936411	-527.899596
BH*and*HLYP/6-311++G(d,p)~LANL2DZ	-528.016343	-527.982887	-528.002740	-527.970626	-528.058152	-528.022046
BH*and*HLYP/aug-*cc*-pVDZ~SDD	-527.970347	-527.938130	-527.956711	-527.925824	-528.012292	-527.977337
BH*and*HLYP/ aug-*cc*-pVDZ~LANL2DZ	-527.946946	-527.914533	-527.933304	-527.902228	-527.988886	-527.953737
BH*and*HLYP/6-311++G(d,p)~def2-TZVP	-814.340519	-814.307880	-814.326904	-814.295613	-814.382477	-814.347049
BH*and*HLYP/aug-*cc*-pVDZ~def2-TZVP	-814.268983	-814.236914	-814.255382	-814.224622	-814.310739	-814.276104
B3LYP/6-31+G(d)~SDD	-528.291987	-528.260706	-528.278049	-528.248084	-528.334105	-528.300187
B3LYP/6-311++G(d,p)~SDD	-528.422926	-528.392409	-528.408970	-528.379732	-528.465100	-528.431980
B3LYP/6-31+G(d)~LANL2DZ	-528.260997	-528.229272	-528.247075	-528.216655	-528.303057	-528.268744
B3LYP/6-311++G(d,p)~LANL2DZ	-528.392197	-528.361338	-528.378246	-528.348673	-528.434374	-528.400888
B3LYP/aug-*cc*-pVDZ~SDD	-528.345988	-528.316484	-528.332006	-528.303787	-528.388240	-528.356088
B3LYP/ aug-*cc*-pVDZ~LANL2DZ	-528.315574	-528.285859	-528.301591	-528.273166	-528.357800	-528.325452
B3LYP/6-311++G(d,p)~def2-TZVP	-814.811423	-814.781377	-814.797469	-814.768709	-814.853667	-814.820934
B3LYP/aug-*cc*-pVDZ~def2-TZVP	-814.732768	-814.703430	-814.718811	-814.690751	-814.774874	-814.742990
M052X/6-31+G(d)~SDD	-528.195896	-528.162371	-528.182897	-528.149895	-528.236606	-528.201863
M052X/6-311++G(d,p)~SDD	-528.325039	-528.292533	-528.311221	-528.280054	-528.367318	-528.331969
M052X/6-31+G(d)~LANL2DZ	-528.167156	-528.133330	-528.153292	-528.120866	-528.209969	-528.172789
M052X/6-311++G(d,p)~LANL2DZ	-528.296660	-528.263778	-528.282842	-528.251314	-528.338950	-528.303181
M052X/aug-*cc*-pVDZ~SDD	-528.267034	-528.235176	-528.254021	-528.222682	-528.307379	-528.274724
M052X/aug-*cc*-pVDZ~LANL2DZ	-528.238843	-528.206859	-528.224931	-528.194370	-528.281796	-528.246380

Table S7 Computed electronic total energies with zero-point energy correction (E+ZPVE, in hartree), enthalpies, (H, in hartree), and Gibbs free energies (G, in hartree) for the stationary points **1c** and **TS17c** at different levels of theory

Levels of theory	E+ZPVE		H		G	
	1c	**TS17c**	**1c**	**TS17c**	**1c**	**TS17c**
BH*and*HLYP/6-31+G(d)~SDD	-567.179224	-567.141616	-567.164546	-567.128025	-567.222267	-567.182341
BH*and*HLYP/6-311++G(d,p)~SDD	-567.310270	-567.273650	-567.295549	-567.260046	-567.353406	-567.314364
BH*and*HLYP/6-31+G(d)~LANL2DZ	-567.155039	-567.117107	-567.140371	-567.103527	-567.198045	-567.157809
BH*and*HLYP/6-311++G(d,p)~LANL2DZ	-567.286509	-567.249651	-567.271799	-567.236045	-567.329609	-567.290371
BH*and*HLYP/aug-*cc*-pVDZ~SDD	-567.234049	-567.198297	-567.219308	-567.184650	-567.277153	-567.239090
BH*and*HLYP/ aug-*cc*-pVDZ~LANL2DZ	-567.210668	-567.174752	-567.195925	-567.161103	-567.253763	-567.215538
BH*and*HLYP/6-311++G(d,p)~def2-TZVP	-853.610600	-853.574513	-853.595895	-853.560905	-853.653714	-853.615238
BH*and*HLYP/aug-*cc*-pVDZ~def2-TZVP	-853.532669	-853.497040	-853.517940	-853.483407	-853.575757	-853.537808
B3LYP/6-31+G(d)~SDD	-567.579316	-567.544562	-567.564246	-567.530539	-567.622659	-567.585708
B3LYP/6-311++G(d,p)~SDD	-567.720859	-567.687075	-567.705754	-567.673043	-567.764270	-567.728234
B3LYP/6-31+G(d)~LANL2DZ	-567.548363	-567.513206	-567.533297	-567.499194	-567.591694	-567.554326
B3LYP/6-311++G(d,p)~LANL2DZ	-567.690150	-567.656128	-567.675051	-567.642099	-567.733556	-567.697267
B3LYP/aug-*cc*-pVDZ~SDD	-567.636826	-567.603927	-567.621677	-567.589885	-567.680336	-567.645049
B3LYP/ aug-*cc*-pVDZ~LANL2DZ	-567.606451	-567.573358	-567.591298	-567.559312	-567.649963	-567.614481
B3LYP/6-311++G(d,p)~def2-TZVP	-854.109326	-854.076075	-854.094220	-854.062043	-854.152814	-854.117235
B3LYP/aug-*cc*-pVDZ~def2-TZVP	-854.023607	-853.990861	-854.008461	-853.976827	-854.067174	-854.031969
M052X/6-31+G(d)~SDD	-567.476848	-567.440567	-567.461923	-567.426719	-567.520475	-567.481510
M052X/6-311++G(d,p)~SDD	-567.616874	-567.581517	-567.601920	-567.567651	-567.660743	-567.622500
M052X/6-31+G(d)~LANL2DZ	-567.448176	-567.411636	-567.433269	-567.397800	-567.491670	-567.452538
M052X/6-311++G(d,p)~LANL2DZ	-567.588369	-567.552926	-567.573438	-567.539070	-567.632016	-567.593871
M052X/aug-*cc*-pVDZ~SDD	-567.552602	-567.518216	-567.537609	-567.504342	-567.596600	-567.559273
M052X/aug-*cc*-pVDZ~LANL2DZ	-567.524440	-567.489939	-567.509446	-567.476073	-567.568386	-567.530955

Table S8 Computed electronic total energies with zero-point energy correction (E+ZPVE, in hartree), enthalpies, (H, in hartree), and Gibbs free energies (G, in hartree) for the stationary points **1d** and **TS6d** at different levels of theory

Levels of theory	E+ZPVE		H		G	
	1d	**TS6d**	**1d**	**TS6d**	**1d**	**TS6d**
BH*and*HLYP/6-31+G(d)~SDD	-606.435574	-606.393821	-606.419656	-606.378792	-606.479416	-606.435802
BH*and*HLYP/6-311++G(d,p)~SDD	-606.576908	-606.535972	-606.560951	-606.520881	-606.620816	-606.578065
BH*and*HLYP/6-31+G(d)~LANL2DZ	-606.411638	-606.369611	-606.395725	-606.354587	-606.455467	-606.411572
BH*and*HLYP/6-311++G(d,p)~LANL2DZ	-606.553167	-606.511955	-606.537213	-606.496872	-606.597092	-606.554034
BH*and*HLYP/aug-*cc*-pVDZ~SDD	-606.494376	-606.454284	-606.478391	-606.439150	-606.538271	-606.496457
BH*and*HLYP/aug-*cc*-pVDZ~LANL2DZ	-606.471049	-606.430808	-606.455061	-606.415672	-606.514942	-606.472976
BH*and*HLYP/6-311++G(d,p)~def2-TZVP	-892.877152	-892.836816	-892.861206	-892.821720	-892.921043	-892.878940
BH*and*HLYP/aug-*cc*-pVDZ~def2-TZVP	-892.792951	-892.752993	-892.776977	-892.737869	-892.836857	-892.795160
B3LYP/6-31+G(d)~SDD	-606.862839	-606.823790	-606.846465	-606.808248	-606.907061	-606.866356
B3LYP/6-311++G(d,p)~SDD	-607.015057	-606.976778	-606.998644	-606.961188	-607.059384	-607.019465
B3LYP/6-31+G(d)~LANL2DZ	-606.831919	-606.792596	-606.815547	-606.777054	-606.876135	-606.835152
B3LYP/6-311++G(d,p)~LANL2DZ	-606.984350	-606.945898	-606.967938	-606.930308	-607.028708	-606.988588
B3LYP/aug-*cc*-pVDZ~SDD	-606.924083	-606.886705	-606.907623	-606.871059	-606.968490	-606.929646
B3LYP/ aug-*cc*-pVDZ~LANL2DZ	-606.893751	-606.856214	-606.877284	-606.840566	-606.938185	-606.899142
B3LYP/6-311++G(d,p)~def2-TZVP	-893.403444	-893.365703	-893.387026	-893.350102	-893.447873	-893.408511
B3LYP/aug-*cc*-pVDZ~def2-TZVP	-893.310826	-893.273554	-893.294370	-893.257910	-893.355312	-893.316576
M052X/6-31+G(d)~SDD	-606.756690	-606.715476	-606.740543	-606.700320	-606.800770	-606.757422
M052X/6-311++G(d,p)~SDD	-606.907588	-606.867009	-606.891454	-606.851799	-606.951476	-606.909066
M052X/6-31+G(d)~LANL2DZ	-606.728094	-606.686770	-606.711951	-606.671586	-606.772175	-606.728783
M052X/6-311++G(d,p)~LANL2DZ	-606.879170	-606.838338	-606.863056	-606.823157	-606.922993	-606.880307
M052X/aug-*cc*-pVDZ~SDD	-606.837467	-606.797845	-606.822068	-606.782544	-606.880006	-606.840134
M052X/aug-*cc*-pVDZ~LANL2DZ	-606.809474	-606.769682	-606.794049	-606.754377	-606.852079	-606.811953

Table S9 Computed activation energies with ZPVE correction ($\Delta_rE^{\neq}$, in kcal/mol), activation enthalpies ($\Delta_rH^{\neq}$, in kcal/mol), and activation Gibbs free energies ($\Delta_rG^{\neq}$, in kcal/mol) using the lowest-lying isomer of the substrate as reactant and the dominant atropisomerization TS as the activation TS for systems **B**, **C**, and **D**

Levels of theory	System **B** **1b→→TS5b**			System **C** **1c→→TS17c**			System **D** **1d→→TS6d**		
	$\Delta_rE^{\neq}$	$\Delta_rH^{\neq}$	$\Delta_rG^{\neq}$	$\Delta_rE^{\neq}$	$\Delta_rH^{\neq}$	$\Delta_rG^{\neq}$	$\Delta_rE^{\neq}$	$\Delta_rH^{\neq}$	$\Delta_rG^{\neq}$
BH*and*HLYP/6-31+G(d)~SDD	21.25	20.40	22.91	23.60	22.92	25.05	26.20	25.64	27.37
BH*and*HLYP/6-311++G(d,p)~SDD	20.82	19.97	22.47	22.98	22.28	24.50	25.69	25.14	26.83
BH*and*HLYP/6-31+G(d)~LANL2DZ	21.48	20.64	23.10	23.80	23.12	25.25	26.37	25.81	27.54
BH*and*HLYP/6-311++G(d,p)~LANL2DZ	20.99	20.15	22.66	23.13	22.44	24.62	25.86	25.31	27.02
BH*and*HLYP/aug-*cc*-pVDZ~SDD	20.22	19.38	21.93	22.43	21.75	23.88	25.16	24.62	26.24
BH*and*HLYP/ aug-*cc*-pVDZ~LANL2DZ	20.34	19.50	22.06	22.54	21.85	23.99	25.25	24.72	26.33
BH*and*HLYP/6-311++G(d,p)~def2-TZVP	20.48	19.64	22.23	22.64	21.96	24.14	25.31	24.78	26.42
BH*and*HLYP/aug-*cc*-pVDZ~def2-TZVP	20.12	19.30	21.73	22.36	21.67	23.81	25.07	24.54	26.17
B3LYP/6-311++G(d,p)~def2-TZVP	18.85	18.05	20.54	20.87	20.19	22.33	23.68	23.17	24.70
B3LYP/aug-*cc*-pVDZ~def2-TZVP	18.41	17.61	20.01	20.55	19.85	22.09	23.39	22.88	24.31
B3LYP/6-31+G(d)~SDD	19.63	18.80	21.28	21.81	21.15	23.19	24.50	23.98	25.54
B3LYP/6-311++G(d,p)~SDD	19.15	18.35	20.78	21.20	20.53	22.61	24.02	23.50	25.05
B3LYP/6-31+G(d)~LANL2DZ	19.91	19.09	21.53	22.06	21.40	23.45	24.68	24.15	25.72
B3LYP/6-311++G(d,p)~LANL2DZ	19.36	18.56	21.01	21.35	20.68	22.77	24.13	23.61	25.18
B3LYP/aug-*cc*-pVDZ~SDD	18.51	17.71	20.18	20.64	19.95	22.14	23.46	22.94	24.37
B3LYP/ aug-*cc*-pVDZ~LANL2DZ	18.65	17.84	20.30	20.77	20.07	22.27	23.55	23.04	24.50
M052X/6-31+G(d)~SDD	21.04	20.71	21.80	22.77	22.09	24.45	25.86	25.24	27.20
M052X/6-311++G(d,p)~SDD	20.40	19.56	22.18	22.19	21.50	24.00	25.46	24.88	26.61
M052X/6-31+G(d)~LANL2DZ	21.23	20.35	23.33	22.93	22.26	24.56	25.93	25.33	27.23
M052X/6-311++G(d,p)~LANL2DZ	20.63	19.78	22.45	22.24	21.57	23.94	25.62	25.04	26.79
M052X/aug-*cc*-pVDZ~SDD	19.99	19.67	20.49	21.58	20.88	23.42	24.86	24.80	25.02
M052X/aug-*cc*-pVDZ~LANL2DZ	20.07	19.18	22.22	21.65	20.94	23.49	24.97	24.89	25.18

Table S10 Computed relative activation energies with ZPVE correction ($\Delta\Delta_rE^{\neq}$, in kcal/mol), relative activation enthalpies ($\Delta\Delta_rH^{\neq}$, in kcal/mol), and relative activation Gibbs free energies ($\Delta\Delta_rG^{\neq}$, in kcal/mol) relative to the system **D**

Levels of theory	System **B** **1b→→TS5b**			System **C** **1c→→TS17c**			System **D** **1d→→TS6d**		
	$\Delta\Delta E^{\neq}$	$\Delta\Delta H^{\neq}$	$\Delta\Delta G^{\neq}$	$\Delta\Delta E^{\neq}$	$\Delta\Delta H^{\neq}$	$\Delta\Delta G^{\neq}$	$\Delta\Delta E^{\neq}$	$\Delta\Delta H^{\neq}$	$\Delta\Delta G^{\neq}$
BH*and*HLYP/6-31+G(d)~SDD	-4.95	-5.24	-4.46	-2.60	-2.72	-2.32	0.00	0.00	0.00
BH*and*HLYP/6-311++G(d,p)~SDD	-4.87	-5.17	-4.36	-2.71	-2.86	-2.33	0.00	0.00	0.00
BH*and*HLYP/6-31+G(d)~LANL2DZ	-4.89	-5.17	-4.44	-2.57	-2.69	-2.29	0.00	0.00	0.00
BH*and*HLYP/6-311++G(d,p)~LANL2DZ	-4.87	-5.16	-4.36	-2.73	-2.87	-2.40	0.00	0.00	0.00
BH*and*HLYP/aug-*cc*-pVDZ~SDD	-4.94	-5.24	-4.31	-2.73	-2.87	-2.36	0.00	0.00	0.00
BH*and*HLYP/ aug-*cc*-pVDZ~LANL2DZ	-4.91	-5.22	-4.27	-2.71	-2.87	-2.34	0.00	0.00	0.00
B3LYP/6-31+G(d)~SDD	-4.87	-5.18	-4.26	-2.69	-2.83	-2.35	0.00	0.00	0.00
B3LYP/6-311++G(d,p)~SDD	-4.87	-5.15	-4.27	-2.82	-2.97	-2.44	0.00	0.00	0.00
B3LYP/6-31+G(d)~LANL2DZ	-4.77	-5.06	-4.19	-2.62	-2.75	-2.27	0.00	0.00	0.00
B3LYP/6-311++G(d,p)~LANL2DZ	-4.77	-5.05	-4.17	-2.78	-2.93	-2.41	0.00	0.00	0.00
B3LYP/aug-*cc*-pVDZ~SDD	-4.95	-5.23	-4.19	-2.82	-2.99	-2.23	0.00	0.00	0.00
B3LYP/ aug-*cc*-pVDZ~LANL2DZ	-4.90	-5.20	-4.20	-2.78	-2.97	-2.23	0.00	0.00	0.00
M052X/6-31+G(d)~SDD	-4.82	-4.53	-5.40	-3.09	-3.15	-2.75	0.00	0.00	0.00
M052X/6-311++G(d,p)~SDD	-5.06	-5.32	-4.43	-3.27	-3.38	-2.61	0.00	0.00	0.00
M052X/6-31+G(d)~LANL2DZ	-4.70	-4.98	-3.90	-3.00	-3.07	-2.67	0.00	0.00	0.00
M052X/6-311++G(d,p)~LANL2DZ	-4.99	-5.26	-4.34	-3.38	-3.47	-2.85	0.00	0.00	0.00
M052X/aug-*cc*-pVDZ~SDD	-4.87	-5.13	-4.53	-3.28	-3.92	-1.60	0.00	0.00	0.00
M052X/aug-*cc*-pVDZ~LANL2DZ	-4.90	-5.71	-2.96	-3.32	-3.95	-1.69	0.00	0.00	0.00
BH*and*HLYP/6-311++G(d,p)~def2-TZVP	-4.83	-5.14	-4.19	-2.67	-2.82	-2.28	0.00	0.00	0.00
BH*and*HLYP/aug-*cc*-pVDZ~def2-TZVP	-4.95	-5.24	-4.44	-2.71	-2.87	-2.36	0.00	0.00	0.00
B3LYP/6-311++G(d,p)~def2-TZVP	-4.83	-5.12	-4.16	-2.81	-2.98	-2.37	0.00	0.00	0.00
B3LYP/aug-*cc*-pVDZ~def2-TZVP	-4.98	-5.27	-4.30	-2.84	-3.03	-2.22	0.00	0.00	0.00

Table S11 Computed activation energies with ZPVE correction ($\Delta_rE^{\neq}$, in kcal/mol), activation enthalpies ($\Delta_rH^{\neq}$, in kcal/mol), and activation Gibbs free energies ($\Delta_rG^{\neq}$, in kcal/mol) using the lowest-lying isomer of the substrate as reactant and the dominant atropisomerization TS as the activation TS for system **A**

Levels of theory	System **A** **1a→→TS5a**		
	$\Delta_rE^{\neq}$	$\Delta_rH^{\neq}$	$\Delta_rG^{\neq}$
BH*and*HLYP/6-31+G(d)	20.45	19.53	22.25
BH*and*HLYP/6-311++G(d,p)	18.86	18.00	20.64
BH*and*HLYP/aug-*cc*-pVDZ	18.54	17.68	20.32
B3LYP/6-31+G(d)	18.82	17.95	20.53
B3LYP/6-311++G(d,p)	17.43	16.61	19.16
B3LYP/aug-*cc*-pVDZ	16.96	16.14	18.62
M052X/6-31+G(d)	20.73	20.29	21.84
M052X/6-311++G(d,p)	18.36	17.59	19.88
M052X/aug-*cc*-pVDZ	17.93	17.14	19.46

Table S12 Computed electronic total energies (E, in hartree), zero-point vibrational energies (ZPVE, in hartree/particle), enthalpies (H, in hartree, 383 K), and Gibbs free energies (G, in hartree, 383 K) at the BH*and*HLYP/6-311++G(d,p) level of theory with $C_6H_5CH_3$ as the solvent for the reactant radicals, intermediates, products, and relevant transition states in the cyclization and further reduction reactions of the radical **13a**

Speaies	E	ZPVE	H	G
2a	-517.320212	0.196274	-517.302822	-517.369866
6a	-516.604642	0.180770	-516.586187	-516.659302
7a	-516.599600	0.180656	-516.581157	-516.653295
8a	-516.599549	0.180555	-516.581047	-516.653617
9a	-516.667491	0.180872	-516.649641	-516.718708
10a	-516.645372	0.182459	-516.628748	-516.694363
11a	-516.677761	0.183583	-516.661053	-516.729329
12a	-516.690400	0.183395	-516.673757	-516.740273
3a	-517.317401	0.197998	-517.300890	-517.365765
TS10a (**TS10a′**)	-516.598603	0.180488	-516.581355	-516.649809
TS11a (**TS11a′**)	-516.597599	0.180011	-516.579943	-516.650864
TS12a (**TS12a′**)	-516.596568	0.180755	-516.579202	-516.648548
TS13a (**TS13a′**)	-516.593754	0.181097	-516.576733	-516.644615
TS14a (**TS14a′**)	-516.599790	0.181079	-516.582798	-516.650930
TS15a (**TS15a′**)	-516.601256	0.180034	-516.584085	-516.652015
TS16a (**TS16a′**)	-516.594312	0.180593	-516.577356	-516.644743
TS17a (**TS17a′**)	-516.635549	0.181620	-516.619451	-516.683989
TS18a (**TS18a′**)	-516.635939	0.180621	-516.619444	-516.684831
TS19a (**TS19a′**)	-516.621920	0.181079	-516.605577	-516.670972
TS20a (**TS20a′**)	-993.559254	0.562770	-993.508845	-993.664507
TS21a	-993.569047	0.565375	-993.519592	-993.670758
$HSnBu_3$	-476.902133	0.382192	-476.869920	-476.978144
$SnBu_3$	-476.285901	0.374412	-476.254758	-476.357031

Table S13 Computed electronic total energies (E, in hartree), zero-point vibrational energies (ZPVE, in hartree/particle), enthalpies (H, in hartree, 298.15 K), and Gibbs free energies (G, in hartree, 298.15 K) at the BH*and*HLYP/6-311++G(d,p) level of theory with $C_6H_5CH_3$ as the solvent for the reactant radicals, intermediates, products, and relevant transition states in the cyclization and further reduction reactions of the radical **13b**

Species	E	ZPVE	H	G
2b	-517.320212	0.196274	-517.309103	-517.355774
6b	-516.604642	0.180770	-516.592594	-516.643877
7b	-516.599600	0.180656	-516.587582	-516.638089
8b	-516.599549	0.180555	-516.587477	-516.638316
9b	-516.667491	0.180872	-516.656025	-516.704179
10b	-516.645372	0.182459	-516.634924	-516.680576
11b	-516.677761	0.183583	-516.667154	-516.714942
12b	-516.690400	0.183395	-516.679882	-516.726279
3b	-517.317401	0.197998	-517.306999	-517.352134
TS10b (**TS10b′**)	-516.598603	0.180488	-516.587526	-516.635390
TS11b (**TS11b′**)	-516.597599	0.180011	-516.586124	-516.635898
TS12b (**TS12b′**)	-516.596568	0.180755	-516.585343	-516.633927
TS13b (**TS13b′**)	-516.593754	0.181097	-516.582870	-516.630318
TS14b (**TS14b′**)	-516.599790	0.181079	-516.588924	-516.636577
TS15b (**TS15b′**)	-516.601256	0.180034	-516.590279	-516.637715
TS16b (**TS16b′**)	-516.594312	0.180593	-516.583501	-516.630558
TS17b (**TS17b′**)	-516.635549	0.181620	-516.625434	-516.670417
TS18b (**TS18b′**)	-516.635939	0.180621	-516.625539	-516.671084
TS19b (**TS19b′**)	-516.621920	0.181079	-516.611601	-516.657214
TS20b (**TS20b′**)	-993.559254	0.562770	-993.526271	-993.632135
TS21b	-993.569047	0.565375	-993.536803	-993.639357
$HSnBu_3$	-476.902133	0.382192	-476.880785	-476.955482
$SnBu_3$	-476.285901	0.374412	-476.264819	-476.339372

Table S14 Computed electronic total energies (E, in hartree), zero-point vibrational energies (ZPVE, in hartree/particle), enthalpies (H, in hartree, 298 K), and Gibbs free energies (G, in hartree, 298 K) at the BH*and*HLYP/6-311++G(d,p) level of theory with C_6H_6 as the solvent for the reactant radicals, intermediates, products, and relevant transition states in the cyclization and further reduction reactions of the radical **24c**

Species	E	ZPVE	H	G
2c(1)	-556.589977	0.225622	-556.577633	-556.627482
2c(2)	-556.589958	0.225610	-556.577611	-556.627461
10c	-555.875166	0.210259	-555.862041	-555.915688
11c	-555.870173	0.210052	-555.857017	-555.910225
12c	-555.869030	0.210017	-555.855854	-555.909286
13c	-555.874933	0.210236	-555.861784	-555.915555
14c	-555.869846	0.210021	-555.856665	-555.910037
15c	-555.869376	0.210006	-555.856174	-555.909744
16c	-555.870189	0.210840	-555.857293	-555.910018
17c	-555.871260	0.210552	-555.858259	-555.911418
18c	-555.937286	0.210233	-555.924582	-555.975912
19c	-555.937302	0.210179	-555.924583	-555.975982
20c	-555.914790	0.211904	-555.903137	-555.951796
21c	-555.915167	0.211835	-555.903499	-555.952267
22c	-555.946729	0.212907	-555.934914	-555.984433
23c	-555.959266	0.212692	-555.947466	-555.996917
3c	-556.586436	0.227395	-556.574822	-556.622769
TS23c	-555.851241	0.208992	-555.838611	-555.890942
TS24c	-555.850250	0.209119	-555.837659	-555.889806
TS25c	-555.852231	0.208938	-555.839583	-555.891771
TS26c	-555.851231	0.209075	-555.838635	-555.890582
TS27c	-555.868314	0.210277	-555.856077	-555.906886
TS28c	-555.855221	0.210943	-555.843226	-555.893461
TS29c	-555.857665	0.210310	-555.845376	-555.897456
TS30c	-555.865651	0.210084	-555.853230	-555.905165
TS31c	-555.868089	0.209752	-555.855755	-555.906630
TS32c	-555.867709	0.209508	-555.855149	-555.907396
TS33c	-555.868093	0.209478	-555.855507	-555.908018
TS34c	-555.868331	0.209464	-555.855758	-555.908072
TS35c	-555.866693	0.210243	-555.854373	-555.905527
TS36c	-555.867040	0.210216	-555.854731	-555.905717
TS37c	-555.862890	0.210316	-555.850735	-555.901237
TS38c	-555.862303	0.210095	-555.850011	-555.901598
TS39c	-555.867936	0.209732	-555.855624	-555.906364
TS40c	-555.868606	0.210455	-555.856531	-555.906762
TS41c	-555.864203	0.210178	-555.851868	-555.903851
TS42c	-555.871028	0.210095	-555.858668	-555.910429

TS43c	-555.858924	0.209837	-555.846522	-555.897997
TS44c	-555.865168	0.209888	-555.852796	-555.903929
TS45c	-555.858100	0.209850	-555.845664	-555.897405
TS46c	-555.864786	0.209882	-555.852403	-555.903582
TS47c (TS47c′)	-555.870467	0.209372	-555.858226	-555.908825
TS48c (TS48c′)	-555.870764	0.209363	-555.858518	-555.909147
TS49c (TS49c′)	-555.862738	0.209943	-555.850678	-555.900597
TS50c (TS50c′)	-555.862090	0.209663	-555.849868	-555.900663
TS51c (TS51c′)	-555.892912	0.222386	-555.892913	-555.940644
TS52c (TS52c′)	-555.904982	0.210978	-555.893625	-555.941713
TS53c (TS53c′)	-555.905572	0.210063	-555.893977	-555.942492
TS54c (TS54c′)	-555.905770	0.209994	-555.894149	-555.942822
TS55c (TS55c′)	-555.891695	0.210538	-555.880259	-555.928490
TS56c (TS56c′)	-555.891462	0.210381	-555.879925	-555.928776
TS57c (TS57c′)	-555.930423	0.210269	-555.918604	-555.967579
TS58c (TS58c′)	-555.927392	0.210536	-555.915598	-555.964604
TS59c (TS59c′)	-1032.829092	0.592123	-1032.794860	-1032.904347
TS60c (TS60c′)	-1032.829319	0.591930	-1032.794986	-1032.905798
TS61c (TS61c′)	-1032.837438	0.594695	-1032.803893	-1032.909465
TS62c (TS62c′)	-556.573240	0.227423	-556.562338	-556.609052
TS63c (TS63c′)	-556.572228	0.227392	-556.561446	-556.607558
TS64c (TS64c′)	-556.583009	0.225711	-556.571566	-556.619004
TS65c (TS65c′)	-556.580141	0.225919	-556.568701	-556.616236
$HSnBu_3$	-476.902133	0.382192	-476.880785	-476.955482
$SnBu_3$	-476.285901	0.374412	-476.264819	-476.339372

Table S15 Computed electronic total energies (E, in hartree), zero-point vibrational energies (ZPVE, in hartree/particle), enthalpies (H, in hartree, 296.15 K), and Gibbs free energies (G, in hartree, 296.15 K) at the BH*and*HLYP/6-311++G(d,p) level of theory with C_6H_6 as the solvent for the reactant radicals, intermediates, products, and relevant transition states in the cyclization and further reduction reactions of the radical **26d**

Species	E	ZPVE	H	G
2d(1)	-595.857232	0.254395	-595.843512	-595.896110
2d(2)	-595.856815	0.254320	-595.843109	-595.895913
10d	-595.143488	0.238834	-595.128960	-595.186045
11d	-595.136992	0.238745	-595.122501	-595.178708
12d	-595.137952	0.238537	-595.123361	-595.180131
13d	-595.137695	0.238963	-595.123230	-595.179613
14d	-595.133862	0.239060	-595.119340	-595.175991
15d	-595.141197	0.238845	-595.126691	-595.183275
16d	-595.135867	0.238740	-595.121383	-595.177194
17d	-595.136160	0.238682	-595.121656	-595.177607
18d	-595.204513	0.239050	-595.190434	-595.244554
19d	-595.204186	0.238922	-595.190125	-595.244416
20d	-595.181912	0.240849	-595.168961	-595.220124
21d	-595.182014	0.240655	-595.169044	-595.220432
22d	-595.208956	0.241576	-595.195686	-595.248017
23d	-595.210404	0.241659	-595.197309	-595.248948
24d	-595.220947	0.241254	-595.207488	-595.262061
25d	-595.221155	0.241055	-595.208674	-595.259602
3d(1)	-595.850079	0.256002	-595.837004	-595.888044
3d(2)	-595.851076	0.256042	-595.838090	-595.888858
TS22d (**TS22d′**)	-595.136546	0.238110	-595.122633	-595.177978
TS23d (**TS23d′**)	-595.134461	0.238116	-595.120559	-595.175641
TS24d (**TS24d′**)	-595.136740	0.238102	-595.122834	-595.177861
TS25d (**TS25d′**)	-595.134337	0.238016	-595.120359	-595.175643
TS26d (**TS26d′**)	-595.134973	0.238981	-595.121400	-595.174992
TS27d (**TS27d′**)	-595.132903	0.238790	-595.119189	-595.173365
TS28d (**TS28d′**)	-595.115919	0.237707	-595.102071	-595.157008
TS29d (**TS29d′**)	-595.121874	0.238853	-595.108289	-595.162669
TS30d (**TS30d′**)	-595.122788	0.238867	-595.109215	-595.163340
TS31d (**TS31d′**)	-595.171963	0.239640	-595.159274	-595.209922
TS32d (**TS32d′**)	-595.172673	0.238755	-595.159716	-595.211221
TS33d (**TS33d′**)	-595.159335	0.239163	-595.146510	-595.197725
TS34d (**TS34d′**)	-595.130704	0.238963	-595.117217	-595.171106
TS35d (**TS35d′**)	-595.130977	0.239053	-595.117525	-595.171180
TS36d (**TS36d′**)	-595.124513	0.238646	-595.110958	-595.164641
TS37d (**TS37d′**)	-595.124077	0.238473	-595.110399	-595.164766

TS38d (**TS38d′**)	-595.124729	0.238513	-595.111094	-595.165092
TS39d (**TS39d′**)	-595.125426	0.238517	-595.111845	-595.165719
TS40d	-595.133601	0.238972	-595.120070	-595.173312
TS41d	-595.130619	0.239206	-595.117038	-595.170281
TS42d	-595.130736	0.238836	-595.116878	-595.172287
TS43d	-595.129215	0.239287	-595.115605	-595.169681
TS44d	-595.119788	0.237798	-595.105898	-595.160441
TS45d	-595.119212	0.238106	-595.105448	-595.159592
TS46d	-595.119346	0.237572	-595.105334	-595.160477
TS47d	-595.116271	0.237676	-595.102187	-595.157589
TS48d	-595.127212	0.238971	-595.113743	-595.166541
TS49d	-595.131354	0.238792	-595.117730	-595.171274
TS50d	-595.127856	0.238894	-595.114340	-595.167510
TS51d	-595.132953	0.238944	-595.119468	-595.172502
TS52d (**TS52d′**)	-595.134698	0.238138	-595.121041	-595.174547
TS53d (**TS53d′**)	-595.135254	0.238077	-595.121640	-595.175223
TS54d (**TS54d′**)	-595.127003	0.238320	-595.113467	-595.166382
TS55d (**TS55d′**)	-595.128173	0.238393	-595.114666	-595.167543
TS56d (**TS56d′**)	-595.159480	0.251478	-595.158535	-595.209381
TS57d (**TS57d′**)	-595.172861	0.238910	-595.159918	-595.211150
TS58d (**TS58d′**)	-595.171963	0.239640	-595.159274	-595.209922
TS59d (**TS59d′**)	-595.172673	0.238755	-595.159716	-595.211221
TS60d (**TS60d′**)	-595.158222	0.239258	-595.145365	-595.196680
TS61d (**TS61d′**)	-595.159335	0.239163	-595.146510	-595.197725
TS62d (**TS62d′**)	-595.204632	0.240927	-595.192344	-595.242150
TS63d (**TS63d′**)	-595.194056	0.241079	-595.181930	-595.231682
TS64d (**TS64d′**)	-595.188877	0.239106	-595.175757	-595.227706
TS65d (**TS65d′**)	-595.188732	0.239405	-595.175700	-595.227254
TS66d (**TS66d′**)	-595.183767	0.241139	-595.171591	-595.221206
TS67d (**TS67d′**)	-595.196869	0.241462	-595.184674	-595.234050
TS68d (**TS68d′**)	-1072.096117	0.621064	-1072.060583	-1072.171883
TS69d (**TS69d′**)	-1072.094694	0.620244	-1072.060257	-1072.163526
TS70d (**TS70d′**)	-1072.100800	0.623411	-1072.065838	-1072.173832
TS71d (**TS71d′**)	-1072.102148	0.623144	-1072.067936	-1072.173842
TS72d (**TS72d′**)	-595.841679	0.254578	-595.828954	-595.879225
TS73d (**TS73d′**)	-595.841179	0.254760	-595.828487	-595.878680
TS74d (**TS74d′**)	-595.827742	0.255973	-595.815816	-595.864175
TS75d (**TS75d′**)	-595.837976	0.255714	-595.825870	-595.874461
$HSnBu_3$	-476.902073	0.382215	-476.880728	-476.955412
$SnBu_3$	-476.285858	0.374432	-476.264777	-476.339328

Table S16 Computed relative enthalpies (ΔH, in kcal/mol, 383 K) and relative Gibbs free energies (ΔG, in kcal/mol, 383 K) for the reactant radicals, intermediates, and relevant transition states in the cyclization reactions of the radical **6a** with the lowest-lying reactant radical **6a** as the reference zero point

Species	ΔH	ΔG
6a	0.00	0.00
7a	3.16	3.77
8a	3.23	3.57
9a	-39.82	-37.28
10a (**10a′**)	-26.71	-22.00
11a	-46.98	-43.94
12a	-54.95	-50.81
TS10a (**TS10a′**)	3.03	5.96
TS11a (**TS11a′**)	3.92	5.29
TS12a (**TS12a′**)	4.38	6.75
TS13a (**TS13a′**)	5.93	9.22
TS14a (**TS14a′**)	2.13	5.25
TS15a (**TS15a′**)	1.32	4.57
TS16a (**TS16a′**)	5.54	9.14
TS17a (**TS17a′**)	-20.87	-15.49
TS18a (**TS18a′**)	-20.87	-16.02
TS19a (**TS19a′**)	-12.17	-7.32

Table S17 Computed relative enthalpies (ΔH, in kcal/mol, 298 K) and relative Gibbs free energies (ΔG, in kcal/mol, 298 K) for the reactant radicals, intermediates, and relevant transition states in the cyclization reactions of the radical **6b** with the lowest-lying reactant radical **6b** as the reference zero point

Species	ΔH	ΔG
6b	0.00	0.00
7b	3.15	3.63
8b	3.21	3.49
9b	-39.80	-37.84
10b (**10b′**)	-26.56	-23.03
11b	-46.79	-44.59
12b	-54.77	-51.71
TS10b (**TS10b′**)	3.18	5.33
TS11b (**TS11b′**)	4.06	5.01
TS12b (**TS12b′**)	4.55	6.24
TS13b (**TS13b′**)	6.10	8.51
TS14b (**TS14b′**)	2.30	4.58
TS15b (**TS15b′**)	1.45	3.87
TS16b (**TS16b′**)	5.71	8.36
TS17b (**TS17b′**)	-20.61	-16.65
TS18b (**TS18b′**)	-20.67	-17.07
TS19b (**TS19b′**)	-11.93	-8.37

Table S18 Computed relative enthalpies (ΔH, in kcal/mol, 298.15 K) and relative Gibbs free energies (ΔG, in kcal/mol, 298.15 K) for the reactant radicals, intermediates, and relevant transition states in the cyclization reactions of the radical **10c** with the lowest-lying reactant radical **10c** as the reference zero point

Species	ΔH	ΔG
10c	0.00	0.00
11c	3.15	3.43
12c	3.88	4.02
13c	0.16	0.08
14c	3.37	3.55
15c	3.68	3.73
16c	2.98	3.56
17c	2.37	2.68
18c	-39.25	-37.79
19c	-39.25	-37.84
20c	-25.79	-22.66
21c	-26.02	-22.95
22c	-45.73	-43.14
23c	-53.60	-50.97
TS23c	14.70	15.53
TS24c	15.30	16.24
TS25c	14.09	15.01
TS26c	14.69	15.75
TS27c	3.74	5.52
TS28c	11.81	13.95
TS29c	10.46	11.44
TS30c	5.53	6.60
TS31c	3.94	5.68
TS32c	4.32	5.20
TS33c	4.10	4.81
TS34c	3.94	4.78
TS35c	4.81	6.38
TS36c	4.59	6.26
TS37c	7.09	9.07
TS38c	7.55	8.84
TS39c	4.03	5.85
TS40c	3.46	5.60
TS41c	6.38	7.43
TS42c	2.12	3.30
TS43c	9.74	11.10
TS44c	5.80	7.38
TS45c	10.28	11.47
TS46c	6.05	7.60

TS47c (**TS47c′**)	2.39	4.31
TS48c (**TS48c′**)	2.21	4.10
TS49c (**TS49c′**)	7.13	9.47
TS50c (**TS50c′**)	7.64	9.43
TS51c (**TS51c′**)	-19.37	-15.66
TS52c (**TS52c′**)	-19.82	-16.33
TS53c (**TS53c′**)	-20.04	-16.82
TS54c (**TS54c′**)	-20.15	-17.03
TS55c (**TS55c′**)	-11.43	-8.03
TS56c (**TS56c′**)	-11.22	-8.21
TS57c (**TS57c′**)	-35.49	-32.56
TS58c (**TS58c′**)	-33.61	-30.70

Table S19 Computed relative enthalpies (ΔH, in kcal/mol, 296 K) and relative Gibbs free energies (ΔG, in kcal/mol, 296 K) for the reactant radicals, intermediates, and relevant transition states in the cyclization reactions of the radical **10d** with the lowest-lying reactant radical **10d** as the reference zero point

Species	ΔH	ΔG
10d	0.00	0.00
11d	4.05	4.60
12d	3.51	3.71
13d	3.60	4.04
14d	6.04	6.31
15d	1.42	1.74
16d	4.75	5.55
17d	4.58	5.29
TS22d (**TS22d′**)	3.97	5.06
TS23d (**TS23d′**)	5.27	6.53
TS24d (**TS24d′**)	3.84	5.13
TS25d (**TS25d′**)	5.40	6.54
TS26d (**TS26d′**)	4.74	6.94
TS27d (**TS27d′**)	6.13	7.96
TS28d (**TS28d′**)	16.87	18.22
TS29d (**TS29d′**)	12.97	14.67
TS30d (**TS30d′**)	12.39	14.25
TS34d (**TS34d′**)	7.37	9.37
TS35d (**TS35d′**)	7.18	9.33
TS36d (**TS36d′**)	11.30	13.43
TS37d (**TS37d′**)	11.65	13.35
TS38d (**TS38d′**)	11.21	13.15
TS39d (**TS39d′**)	10.74	12.75
TS40d	5.58	7.99
TS41d	7.48	9.89
TS42d	7.58	8.63
TS43d	8.38	10.27
TS44d	14.47	16.07
TS45d	14.75	16.60
TS46d	14.83	16.04
TS47d	16.80	17.86
TS48d	9.55	12.24
TS49d	7.05	9.27
TS50d	9.17	11.63
TS51d	5.96	8.50

Table S20 Computed relative enthalpies (ΔH, in kcal/mol, 383 K) and relative Gibbs free energies (ΔG, in kcal/mol, 383 K) for the reactant radicals, intermediates, products, and relevant transition states in the reduction reactions of the radicals **9a** and **11a** with (*R*)-**9a**+$HSnBu_3$ as the reference zero point

Species	ΔH	ΔG
9a+$HSnBu_3$	0.00	0.00
10a (**10a′**)+$HSnBu_3$	13.11	15.28
11a+$HSnBu_3$	-7.16	-6.66
TS17a (**TS17a′**)+$HSnBu_3$	18.94	21.79
TS18a (**TS18a′**)+$HSnBu_3$	18.95	21.26
TS20a(**TS20a′**)	6.72	20.30
TS21a	-0.02	16.37
2a+$SnBu_3$	-23.86	-18.85
3a+$SnBu_3$	-22.64	-16.28

Table S21 Computed relative enthalpies (ΔH, in kcal/mol, 298.15 K) and relative Gibbs free energies (ΔG, in kcal/mol, 298.15 K) for the reactant radicals, intermediates, products, and relevant transition states in the reduction reactions of the radicals **9b** and **11b** with (*R*)-**9b**+$HSnBu_3$ as the reference zero point

Species	ΔH	ΔG
9b+$HSnBu_3$	0.00	0.00
10b (**10b′**)+$HSnBu_3$	13.24	14.81
11b+$HSnBu_3$	-6.98	-6.75
TS17b (**TS17b′**)+$HSnBu_3$	19.20	21.19
TS18b (**TS18b′**)+$HSnBu_3$	19.13	20.77
TS20b (**TS20b′**)	6.61	17.27
TS21b	0.00	12.74
2b+$SnBu_3$	-23.29	-22.27
3b+$SnBu_3$	-21.97	-19.98

Table S22 Computed relative enthalpies (ΔH, in kcal/mol, 296.15 K) and relative Gibbs free energies (ΔG, in kcal/mol, 296.15 K) for the reactant radicals, intermediates, products, and relevant transition states in the reduction reactions of the radicals **19c** and **22c** with (*R*)-**19c**+$HSnBu_3$ as the reference zero point

Species	ΔH	ΔG
19c+$HSnBu_3$	0.00	0.00
18c+$HSnBu_3$	0.00	0.04
20c+$HSnBu_3$	13.46	15.18
21c+$HSnBu_3$	13.23	14.88
22c+$HSnBu_3$	-6.48	-5.30
TS51c+$HSnBu_3$	19.87	22.17
TS52c+$HSnBu_3$	19.43	21.50
TS53c+$HSnBu_3$	19.21	21.02
TS54c+$HSnBu_3$	19.10	20.81
TS57c+$HSnBu_3$	3.75	5.27
TS58c+$HSnBu_3$	5.64	7.14
TS59c	6.59	17.02
TS60c	6.51	16.11
TS61c	0.93	13.80
TS62c	-13.67	-10.64
TS63c	-13.11	-9.71
TS64c	-19.46	-16.89
TS65c	-17.67	-15.15
2c-1+$SnBu_3$	-23.27	-22.21
2c-2+$SnBu_3$	-23.26	-22.19
22c+$SnBu_3$	-21.51	-19.25

Table S23 Computed relative enthalpies (ΔH, in kcal/mol, 296 K) and relative Gibbs free energies (ΔG, in kcal/mol, 296 K) for the reactant radicals, intermediates, products, and relevant transition states in the reduction reactions of the radicals **18d** and **22d** with (*R*)-**18d**+$HSnBu_3$ as the reference zero point

Species	ΔH	ΔG
18d+$HSnBu_3$	0.00	0.00
2d(1)+$SnBu_3$	-23.30	-22.26
2d(2)+$SnBu_3$	-23.04	-22.14
10d+$HSnBu_3$	38.58	36.71
12d+$HSnBu_3$	42.09	40.43
15d+$HSnBu_3$	40.00	38.45
17d+$HSnBu_3$	43.16	42.01
19d+$HSnBu_3$	0.19	0.09
20d+$HSnBu_3$	13.47	15.33
21d+$HSnBu_3$	13.42	15.14
22d+$HSnBu_3$	-3.30	-2.17
23d+$HSnBu_3$	-4.31	-2.76
24d+$HSnBu_3$	-10.70	-10.99
25d+$HSnBu_3$	-11.45	-9.44
3d(1)+$SnBu_3$	-19.21	-17.20
3d(2)+$SnBu_3$	-19.90	-17.71
TS24d+$HSnBu_3$	42.42	41.85
TS25d+$HSnBu_3$	43.97	43.24
TS34d+$HSnBu_3$	45.94	46.09
TS35d+$HSnBu_3$	45.75	46.04
TS38d+$HSnBu_3$	49.79	49.86
TS39d+$HSnBu_3$	49.32	49.47
TS52d+$HSnBu_3$	43.54	43.93
TS53d+$HSnBu_3$	43.17	43.51
TS54d+$HSnBu_3$	48.30	49.05
TS55d+$HSnBu_3$	47.55	48.33
TS56d+$HSnBu_3$	20.02	22.07
TS57d+$HSnBu_3$	19.15	20.96
TS58d+$HSnBu_3$	19.55	21.73
TS59d+$HSnBu_3$	19.28	20.92
TS60d+$HSnBu_3$	28.28	30.04
TS61d+$HSnBu_3$	27.56	29.39
TS62d+$HSnBu_3$	-1.20	1.51
TS63d+$HSnBu_3$	5.34	8.08
TS64d+$HSnBu_3$	9.21	10.57
TS65d+$HSnBu_3$	9.25	10.86
TS66d+$HSnBu_3$	11.82	14.65
TS67d+$HSnBu_3$	3.61	6.59

TS68d	6.64	17.62
TS69d	6.84	22.87
TS70d	3.34	16.40
TS71d	2.02	16.39
TS72d+$HSnBu_3$	-14.16	-11.66
TS73d+$HSnBu_3$	-13.87	-11.32
TS74d+$HSnBu_3$	-5.92	-2.22
TS75d+$HSnBu_3$	-12.23	-8.67

Details of numerical simulation computation

Figure S15 gave the schematic pathways of radical reactant isomerizations, cyclizations, neophyl-like rearrangements, and reduced radical trappings for the systems **A** and **C**, in which the kinetic rate constants of all elementary reaction steps were named in detail. For the listed elementary reactions in Figure S15, the simultaneous kinetic differential equations are as follows:

$$\frac{\mathrm{d}[(M)\text{-}\mathbf{6}]}{\mathrm{d}t} = -(k_1 + k_6 + k_8 + k_9)[(M)\text{-}\mathbf{6}] + k_7[(M)\text{-}\mathbf{7}] + k_4[(M)\text{-}\mathbf{8}] + k_2'[(P)\text{-}\mathbf{8}] + k_{18}[(R)\text{-}\mathbf{9}]$$

$$\frac{\mathrm{d}[(M)\text{-}\mathbf{7}]}{\mathrm{d}t} = k_8[(M)\text{-}\mathbf{6}] - (k_5 + k_7)[(M)\text{-}\mathbf{7}] + k_3[(M)\text{-}\mathbf{8}]$$

$$\frac{\mathrm{d}[(M)\text{-}\mathbf{8}]}{\mathrm{d}t} = k_6[(M)\text{-}\mathbf{6}] + k_5[(M)\text{-}\mathbf{7}] - (k_2 + k_3 + k_4 + k_{19})[(M)\text{-}\mathbf{8}] + k_9'[(P)\text{-}\mathbf{6}] + k_{20}[\mathbf{11}]$$

$$\frac{\mathrm{d}[(P)\text{-}\mathbf{6}]}{\mathrm{d}t} = k_2[(M)\text{-}\mathbf{8}] - (k_1' + k_6' + k_8' + k_9')[(P)\text{-}\mathbf{6}] + k_7'[(P)\text{-}\mathbf{7}] + k_4'[(P)\text{-}\mathbf{8}] + k_{18}'[(S)\text{-}\mathbf{9}]$$

$$\frac{\mathrm{d}[(P)\text{-}\mathbf{7}]}{\mathrm{d}t} = k_8'[(P)\text{-}\mathbf{6}] - (k_5' + k_7')[(P)\text{-}\mathbf{7}] + k_3'[(P)\text{-}\mathbf{8}]$$

$$\frac{\mathrm{d}[(P)\text{-}\mathbf{8}]}{\mathrm{d}t} = k_9[(M)\text{-}\mathbf{6}] + k_6'[(P)\text{-}\mathbf{6}] + k_5'[(P)\text{-}\mathbf{7}] - (k_2' + k_3' + k_4' + k_{19}')[(P)\text{-}\mathbf{8}] + k_{20}'[\mathbf{11}]$$

$$\frac{\mathrm{d}[\mathbf{10}]}{\mathrm{d}t} = -(k_{13} + k_{14})[\mathbf{10}] + k_{12}[(R)\text{-}\mathbf{9}] + k_{15}[\mathbf{11}]$$

$$\frac{\mathrm{d}[\mathbf{10}']}{\mathrm{d}t} = -(k_{13}' + k_{14}')[\mathbf{10}'] + k_{12}'[(S)\text{-}\mathbf{9}] + k_{15}'[\mathbf{11}]$$

$$\frac{\mathrm{d}[(R)\text{-}\mathbf{9}]}{\mathrm{d}t} = k_1[(M)\text{-}\mathbf{6}] + k_{13}[\mathbf{10}] - (k_{12} + k_{18} + k_{11}[\mathrm{HSnBu_3}])[(R)\text{-}\mathbf{9}] + k_{10}[(R)\text{-}\mathbf{2}][\mathrm{SnBu_3}]$$

$$\frac{\mathrm{d}[(S)\text{-}\mathbf{9}]}{\mathrm{d}t} = k_1'[(P)\text{-}\mathbf{6}] + k_{13}'[\mathbf{10}'] - (k_{12}' + k_{18}' + k_{11}'[\mathrm{HSnBu_3}])[(S)\text{-}\mathbf{9}] + k_{10}'[(S)\text{-}\mathbf{2}][\mathrm{SnBu_3}]$$

$$\frac{\mathrm{d}[\mathbf{11}]}{\mathrm{d}t} = k_{14}[\mathbf{10}] + k_{14}'[\mathbf{10}'] - (k_{15} + k_{15}' + k_{20} + k_{20}' + k_{16}[\mathrm{HSnBu_3}])[\mathbf{11}] + k_{17}[\mathbf{13}][\mathrm{SnBu_3}] + k_{19}[(M)\text{-}\mathbf{8}] + k_{19}'[(P)\text{-}\mathbf{8}]$$

$$\frac{\mathrm{d}[\mathbf{13}]}{\mathrm{d}t} = k_{16}[\mathrm{HSnBu_3}][\mathbf{11}] - k_{17}[\mathbf{13}][\mathrm{SnBu_3}]$$

$$\frac{\mathrm{d}[(R)\text{-}\mathbf{2}]}{\mathrm{d}t} = k_{11}[\mathrm{HSnBu_3}][(R)\text{-}\mathbf{9}] - k_{10}[(R)\text{-}\mathbf{2}][\mathrm{SnBu_3}]$$

$$\frac{\mathrm{d}[(S)\text{-}\mathbf{2}]}{\mathrm{d}t} = k_{11}'[\mathrm{HSnBu_3}][(S)\text{-}\mathbf{9}] - k_{10}'[(S)\text{-}\mathbf{2}][\mathrm{SnBu_3}]$$

For all of the stationary points on the potential energy profiles, we performed thermal corrections at the temperature points selected based on the temperature range from the melting point to the boiling point of the used solvent. The corrected Gibbs free energies were listed in Tables S24 and S25, while the computed rate constants of all elementary reactions using the traditional transition state theory (TST) were given in Tables S26.

In the numerical simulations, the initial reactant concentration $[(M)\text{-}\mathbf{10}]_0$ was set as 1 and $HSnBu_3$ was 1.1 *equiv* of (*M*)-**10**, and the initial concentrations of the remaining species are zero. Using the kinetic differential equations and the mass conservation equations, we wrote a script code based on the MATLAB environment. Further simulation tests on MATLAB (Version R2016b) platform gave the concentration distribution of radical intermediates and the branching ratios of the final cyclization

products. Furthermore, the systems **B** and **D** were computed using the similar methods and steps.

Table S24 Corrected Gibbs free energies (in hartree) of the stationary points on the cyclization reaction profile of the systems **A**/**B** at different temperatures (T, K) and the BH*and*HLYP/6-311++G(d,p) level of theory

Species	178.15	195.15	223.15	248.15	273.15	298.15	323.15	343.15	363.15	383.15
6b	-516.624905	-516.627384	-516.631621	-516.635561	-516.639648	-516.643877	-516.648247	-516.651844	-516.655529	-516.659302
8b	-516.619532	-516.621982	-516.626175	-516.630076	-516.634124	-516.638316	-516.642649	-516.646217	-516.649874	-516.653617
7b	-516.619436	-516.621869	-516.626030	-516.629905	-516.633925	-516.638089	-516.642394	-516.645940	-516.649573	-516.653295
9b	-516.686448	-516.688754	-516.692704	-516.696386	-516.700211	-516.704179	-516.708286	-516.711672	-516.715147	-516.718708
10b (**10b′**)	-516.663751	-516.665945	-516.669696	-516.673188	-516.676815	-516.680576	-516.684471	-516.687683	-516.690981	-516.694363
11b	-516.697250	-516.699567	-516.703521	-516.707194	-516.711002	-516.714942	-516.719015	-516.722369	-516.725807	-516.729329
2b	-517.338598	-517.340831	-517.344657	-517.348223	-517.351929	-517.355774	-517.359756	-517.363039	-517.366410	-517.369866
3b	-517.335502	-517.337670	-517.341377	-517.344830	-517.348416	-517.352134	-517.355985	-517.359161	-517.362421	-517.365765
TS10b (**TS10b′**)	-516.617713	-516.620020	-516.623964	-516.627635	-516.631444	-516.635390	-516.639471	-516.642832	-516.646278	-516.649809
TS11b (**TS11b′**)	-516.617464	-516.619876	-516.623995	-516.627824	-516.631792	-516.635898	-516.640139	-516.643629	-516.647204	-516.650864
TS12b (**TS12b′**)	-516.615954	-516.618303	-516.622318	-516.626050	-516.629920	-516.633927	-516.638068	-516.641475	-516.644974	-516.648548
TS14b (**TS14b′**)	-516.618965	-516.621266	-516.625198	-516.628855	-516.632648	-516.636577	-516.640639	-516.643985	-516.647416	-516.650930
TS15b (**TS15b′**)	-516.620212	-516.622494	-516.626398	-516.630033	-516.633805	-516.637715	-516.641760	-516.645093	-516.648512	-516.652015
TS16b (**TS16b′**)	-516.613187	-516.615454	-516.619329	-516.622936	-516.626679	-516.630558	-516.634570	-516.637877	-516.641268	-516.644743
TS17b (**TS17b′**)	-516.653812	-516.655981	-516.659686	-516.663133	-516.666710	-516.670417	-516.674253	-516.677416	-516.680661	-516.683989
TS18b (**TS18b′**)	-516.654290	-516.656481	-516.660226	-516.663712	-516.667331	-516.671084	-516.674969	-516.678172	-516.681460	-516.684831
$HSnBu_3$	-476.928306	-476.931788	-476.937798	-476.943442	-476.949339	-476.955482	-476.961864	-476.967141	-476.972568	-476.978144
$SnBu_3$	-476.310132	-476.313389	-476.319022	-476.324321	-476.329865	-476.335647	-476.341663	-476.346641	-476.351764	-476.357031

Table S25 Corrected Gibbs free energies (in hartree) of the stationary points on the reduced radical trapping reaction profile of the systems **A/B** at different temperatures (T, K) and the BH*and*HLYP/6-311++G(d,p) level of theory

Species	178.15	195.15	223.15	248.15	273.15	298.15	323.15	343.15	363.15	383.15
9b+$HSnBu_3$	-993.614754	-993.620542	-993.630502	-993.639828	-993.649550	-993.659661	-993.670150	-993.678813	-993.687715	-993.696852
10b (**10b′**)+$HSnBu_3$	-993.592057	-993.597733	-993.607494	-993.616630	-993.626154	-993.636058	-993.646335	-993.654824	-993.663549	-993.672507
11b+$HSnBu_3$	-993.625556	-993.631355	-993.641319	-993.650636	-993.660341	-993.670424	-993.680879	-993.689510	-993.698375	-993.707473
TS20b (**TS20b′**)	-993.594108	-993.598916	-993.607267	-993.615160	-993.623452	-993.632135	-993.641204	-993.648732	-993.656501	-993.664507
TS21b	-993.602587	-993.607228	-993.615295	-993.622926	-993.630950	-993.639357	-993.648147	-993.655447	-993.662984	-993.670758
TS17b (**TS17b′**)+$HSnBu_3$	-993.582118	-993.587769	-993.597484	-993.606575	-993.616049	-993.625899	-993.636117	-993.644557	-993.653229	-993.662133
TS18b (**TS18b′**)+$HSnBu_3$	-993.582596	-993.588269	-993.598024	-993.607154	-993.616670	-993.626566	-993.636833	-993.645313	-993.654028	-993.662975
2b+$SnBu_3$	-993.648730	-993.654220	-993.663679	-993.672544	-993.681794	-993.691421	-993.701419	-993.709680	-993.718174	-993.726897
3b+$SnBu_3$	-993.645634	-993.651059	-993.660399	-993.669151	-993.678281	-993.687781	-993.697648	-993.705802	-993.714185	-993.722796

Table S26 Calculated TST rate constant of the elementary steps on the reaction profiles of the system **A**/**B**. The names of rate constants were listed in Supporting Figure S15

	178.15	195.15	223.15	248.15	273.15	298.15	323.15	343.15	363.15	383.15
k_1	1.0096×10^{9}	1.6310×10^{9}	3.0774×10^{9}	4.8240×10^{9}	6.9549×10^{9}	9.4691×10^{9}	1.2305×10^{10}	1.4772×10^{10}	1.7409×10^{10}	2.0162×10^{10}
k_2	1.0018×10^{8}	2.0556×10^{8}	5.2776×10^{8}	1.0218×10^{9}	1.7469×10^{9}	2.7337×10^{9}	3.9863×10^{9}	5.1807×10^{9}	6.5454×10^{9}	8.0602×10^{9}
k_3	7.8362×10^{9}	1.2803×10^{10}	2.4507×10^{10}	3.8512×10^{10}	5.5784×10^{10}	7.5962×10^{10}	9.8583×10^{10}	1.1780×10^{11}	1.3909×10^{11}	1.6001×10^{11}
k_4	1.1586×10^{11}	1.6556×10^{11}	2.6588×10^{11}	3.7143×10^{11}	4.8933×10^{11}	6.1646×10^{11}	7.4992×10^{11}	8.5914×10^{11}	9.7111×10^{11}	1.0833×10^{12}
k_5	6.6100×10^{9}	1.0664×10^{10}	1.9961×10^{10}	3.0980×10^{10}	4.4320×10^{10}	5.9728×10^{10}	7.6838×10^{10}	9.1296×10^{10}	1.0706×10^{11}	1.2271×10^{11}
k_6	7.1395×10^{6}	2.2036×10^{7}	9.7384×10^{7}	2.7793×10^{8}	6.5481×10^{8}	1.3411×10^{9}	2.4602×10^{9}	3.7533×10^{9}	5.4693×10^{9}	7.6661×10^{9}
k_7	1.4837×10^{11}	1.7064×10^{11}	2.0411×10^{11}	2.3202×10^{11}	2.5734×10^{11}	2.8059×10^{11}	3.0207×10^{11}	3.1768×10^{11}	3.3217×10^{11}	3.4641×10^{11}
k_8	1.0839×10^{7}	2.7269×10^{7}	9.1788×10^{7}	2.1582×10^{8}	4.3344×10^{8}	7.7632×10^{8}	1.2714×10^{9}	1.7908×10^{9}	2.4305×10^{9}	3.1965×10^{9}
k_9	1.0018×10^{8}	2.0556×10^{8}	5.2776×10^{8}	1.0218×10^{9}	1.7469×10^{9}	2.7337×10^{9}	3.9863×10^{9}	5.1807×10^{9}	6.5454×10^{9}	8.0602×10^{9}
k_{10}	1.1598×10^{-29}	1.7088×10^{-26}	2.5794×10^{-22}	2.2853×10^{-19}	5.9883×10^{-17}	6.3060×10^{-15}	3.3007×10^{-13}	5.2409×10^{-12}	6.2026×10^{-11}	5.7287×10^{-10}
k_{11}	1.6614×10^{-3}	7.9584×10^{-3}	6.3379×10^{-2}	2.7565×10^{-1}	9.2646×10^{-1}	2.5653	6.1571	1.1377×10	1.9756×10	3.2549×10
k_{12}	5.5081×10^{-13}	6.8494×10^{-11}	3.8446×10^{-8}	3.2538×10^{-6}	1.2174×10^{-4}	2.4709×10^{-3}	3.1424×10^{-2}	1.8393×10^{-1}	8.8435×10^{-1}	3.6129
k_{13}	1.6370×10^{5}	7.3333×10^{5}	5.3146×10^{6}	2.1548×10^{7}	6.7989×10^{7}	1.7786×10^{8}	4.0226×10^{8}	7.1181×10^{8}	1.1834×10^{9}	1.8709×10^{9}
k_{14}	4.2519×10^{5}	1.8161×10^{6}	1.2414×10^{7}	4.8470×10^{7}	1.4876×10^{8}	3.8183×10^{8}	8.5224×10^{8}	1.4954×10^{9}	2.4740×10^{9}	3.8943×10^{9}
k_{15}	6.9137×10^{-21}	4.2694×10^{-18}	2.0194×10^{-14}	7.7824×10^{-12}	1.0172×10^{-9}	5.9394×10^{-8}	1.8615×10^{-6}	2.0501×10^{-5}	1.7420×10^{-4}	1.1871×10^{-3}
k_{16}	3.3323×10^{-5}	1.6957×10^{-4}	1.4685×10^{-3}	6.7933×10^{-3}	2.4026×10^{-2}	6.9542×10^{-2}	1.7362×10^{-1}	3.2959×10^{-1}	5.8649×10^{-1}	9.8908×10^{-1}
k_{17}	1.1639×10^{-20}	2.4090×10^{-18}	2.7568×10^{-15}	3.9742×10^{-13}	2.3611×10^{-11}	7.2135×10^{-10}	1.3266×10^{-8}	1.0152×10^{-7}	6.2729×10^{-7}	3.2391×10^{-6}
k_{18}	4.2255×10^{-39}	1.2106×10^{-34}	8.8481×10^{-29}	1.1662×10^{-24}	2.7162×10^{-21}	1.7290×10^{-18}	4.0656×10^{-16}	1.8111×10^{-14}	5.3147×10^{-13}	1.0975×10^{-11}
k_{19}	6.8127×10^{7}	1.4580×10^{8}	3.9620×10^{8}	7.9779×10^{8}	1.4135×10^{9}	2.2757×10^{9}	3.4016×10^{9}	4.4991×10^{9}	5.7753×10^{9}	7.2153×10^{9}
k_{20}	8.4917×10^{-53}	3.6256×10^{-47}	9.3820×10^{-40}	1.5345×10^{-34}	2.8209×10^{-30}	1.0122×10^{-26}	1.0309×10^{-23}	1.2785×10^{-21}	9.3560×10^{-20}	4.3873×10^{-18}

Table S27 Calculated the concentration distribution (%) of the radical intermediates and the final product for system **A**/**B**

T	[(*M*)-**1a/b**]:[(*P*)-**1a/b**] = 100:0					[(*M*)-**1a/b**]:[(*P*)-**1a/b**] = 75:25					[(*M*)-**1a/b**]:[(*P*)-**1a/b**] = 50:50				
	(*R*)-**9b**	(*S*)-**9b**	(*R*)-**2b**	(*S*)-**2b**	**3b**	(*R*)-**9b**	(*S*)-**9b**	(*R*)-**2b**	(*S*)-**2b**	**3b**	(*R*)-**9b**	(*S*)-**9b**	(*R*)-**2b**	(*S*)-**2b**	**3b**
178	91.7	8.3	91.7	8.3	0	70.9	29.1	70.9	29.1	0	50.0	50.0	50.0	50.0	0
195	89.9	10.1	89.9	10.1	0	70.0	30.0	70.0	30.0	0	50.0	50.0	50.0	50.0	0
223	87.2	12.8	87.2	12.8	0	68.6	31.4	68.6	31.4	0	50.0	50.0	50.0	50.0	0
248	85.1	14.9	85.1	14.9	0	67.6	32.4	67.6	32.4	0	50.0	50.0	50.0	50.0	0
273	83.3	16.7	83.3	16.7	0	66.7	33.3	66.7	33.3	0	50.0	50.0	50.0	50.0	0
298	81.5	18.5	81.4	18.5	0.1	65.8	34.2	65.7	34.2	0.1	50.0	50.0	50.0	50.0	0
323	80.3	19.6	80.0	19.5	0.5	65.2	34.8	64.9	34.6	0.5	50.0	50.0	49.7	49.7	0.6
343	79.4	20.6	78.1	20.3	1.6	64.7	35.3	63.7	34.7	1.6	50.0	50.0	49.2	49.2	1.6
363	78.5	21.5	75.1	20.6	4.3	64.3	35.7	61.5	34.2	4.3	50.0	50.0	47.9	47.9	4.2
383	77.8	22.2	70.0	20.0	10.0	63.9	36.1	57.5	32.5	10.0	50.0	50.0	45.0	45.0	10.0

Table S28 Calculated the concentration distribution (%) of the radical intermediates and the final productsfor the system **C**

T	[(*M*)-**1c**]:[(*P*)-**1c**] = 100:0					[(*M*)-**1c**]:[(*P*)-**1c**] = 75:25					[(*M*)-**1c**]:[(*P*)-**1c**] = 50:50				
	(*R*)-**18c**+ (*R*)-**19c**	(*S*)-**18c**+ (*S*)-**19c**	(*R*)-**2c(1)**+ (*R*)-**2c(2)**	(*S*)-**2c(1)**+ (*S*)-**2c(2)**	**3c**	(*R*)-**18c**+ (*R*)-**19c**	(*S*)-**18c**+ (*S*)-**19c**	(*R*)-**2c(1)**+ (*R*)-**2c(2)**	(*S*)-**2c(1)**+ (*S*)-**2c(2)**	**3c**	(*R*)-**18c**+ (*R*)-**19c**	(*S*)-**18c**+ (*S*)-**19c**	(*R*)-**2c(1)**+ (*R*)-**2c(2)**	(*S*)-**2c(1)**+ (*S*)-**2c(2)**	**3c**
178	97.4	2.6	97.4	2.6	0	73.4	26.6	73.4	26.6	0	49.5	50.5	49.5	50.5	0
195	96.3	3.7	96.3	3.7	0	72.8	27.2	72.8	27.2	0	49.3	50.7	49.3	50.7	0
223	94.3	5.7	94.3	5.7	0	71.7	28.3	71.7	28.3	0	49.0	51.0	49.0	51.0	0
248	92.4	7.6	92.4	7.6	0	70.6	29.4	70.6	29.4	0	48.7	51.3	48.7	51.3	0
273	90.4	9.6	90.4	9.6	0	69.5	30.5	69.5	30.5	0	48.5	51.5	48.5	51.5	0
298	88.6	11.4	88.6	11.4	0	68.5	31.5	68.5	31.5	0	48.3	51.7	48.3	51.7	0
323	86.8	13.2	86.7	13.2	0.1	67.5	32.5	67.4	32.5	0.1	48.2	51.8	48.2	51.7	0.1
343	85.4	14.6	85.2	14.6	0.2	66.8	33.2	66.7	33.1	0.2	48.1	51.9	48.0	51.8	0.2
363	84.2	15.8	83.6	15.7	0.7	66.1	33.9	65.6	33.7	0.7	48.0	52.0	47.7	51.6	0.7
383	83.0	17.0	81.6	16.7	1.7	65.5	34.5	64.4	33.9	1.7	48.0	52.0	47.2	51.1	1.7

Table S29 Calculated the concentration distribution (%) of the radical intermediates and products with different *M*-to-*P* ratio of the initial reactant **1d**

T	[(*M*)-**1d**]:[(*P*)-**1d**] = 100:0					[(*M*)-**1d**]:[(*P*)-**1d**] = 83:17				
	(*R*)-**18d**+ (*R*)-**19d**	(*S*)-**18d**+ (*S*)-**19d**	(*R*)-**2d-1**+ (*R*)-**2d-2**	(*S*)-**2d-1**+ (*S*)-**2d-2**	**3d(1)**+ **3d(2)**	(*R*)-**18d**+ (*R*)-**19d**	(*S*)-**18d**+ (*S*)-**19d**	(*R*)-**2d-1**+ (*R*)-**2d-2**	(*S*)-**2d-1**+ (*S*)-**2d-2**	**3d(1)**+ **3d(2)**
279	95.7	4.3	95.7	4.3	0	80.1	19.9	80.1	19.9	0
298	94.6	5.4	94.6	5.4	0	79.4	20.6	79.4	20.6	0
313	93.7	6.3	93.6	6.3	0.1	78.9	21.1	78.8	21.1	0.1
323	93.1	6.9	92.9	6.9	0.2	78.5	21.5	78.3	21.5	0.2
333	92.5	7.5	92.1	7.5	0.4	78.1	21.9	77.7	21.8	0.5
343	91.9	8.1	91.2	8.0	0.8	77.7	22.3	77.1	22.1	0.8
353	91.3	8.7	90.1	8.6	1.3	77.3	22.7	76.2	22.4	1.4
	[(*M*)-**1d**]:[(*P*)-**1d**] = 50:50					[(*M*)-**1d**]:[(*P*)-**1d**] = 14:86				
279	50.0	50.0	50.0	50.0	0	17.1	82.9	17.1	82.9	0.0
298	50.0	50.0	50.0	50.0	0	17.9	82.1	17.9	82.1	0.0
313	50.0	50.0	50.0	50.0	0	18.5	81.5	18.5	81.4	0.1
323	50.0	50.0	49.9	49.9	0.2	18.9	81.1	18.9	80.9	0.2
333	50.0	50.0	49.8	49.8	0.4	19.4	81.6	19.3	80.2	0.5
343	50.0	50.0	49.6	49.6	0.8	19.8	80.2	19.6	79.6	0.8
353	50.0	50.0	49.3	49.3	1.4	20.3	79.7	20.0	78.6	1.4

Table S30 Calculated concentration ratio ([**2d**]/[**1d**]) and chirality transfer ratio (CTR), *i.e. ee* (product)/*ee* (subtrate), in which *ee* (product) and *ee* (subtrate) refer to the enantiomeric excesses of product and substrate, respectively, at different temperatures (T, K) for system **D**

T	[(*M*)-**1d**]:[(*P*)-**1d**] = 100:0		[(*M*)-**1d**]:[(*P*)-**1d**] = 83:17		[(*M*)-**1d**]:[(*P*)-**1d**] = 14:86		Average value of CTR
	[(*R*)-**2d**]/[(*M*)-**1d**]	CTR	[(*R*)-**2d**]/[(*M*)-**1d**]	CTR	[(*S*)-**2d**]/[(*P*)-**1d**]	CTR	
279	0.957	0.914	0.965	0.912	0.964	0.914	0.913
298	0.946	0.892	0.957	0.891	0.955	0.892	0.892
313	0.936	0.874	0.949	0.875	0.947	0.874	0.874
323	0.929	0.862	0.943	0.862	0.941	0.863	0.862
333	0.921	0.849	0.936	0.851	0.933	0.850	0.850
343	0.912	0.839	0.929	0.840	0.926	0.840	0.840
353	0.901	0.826	0.918	0.827	0.914	0.825	0.826

Table S31 Geometries in Cartesian coordinates of the optimized cyclization and reduction transition states at the BH*and*HLYP/6-311++G(d,p)~SDD level of theory

Species	Geometries	Species	Geometries
TS15a	6 -1.899347 1.568153 -0.063108	**TS16a**	6 -2.183588 1.324783 0.031151
	6 -3.052662 0.784091 -0.062976		6 -3.140663 0.334068 -0.164204
	6 -2.938505 -0.593922 -0.013722		6 -2.735008 -0.986258 -0.234860
	6 -1.698853 -1.217814 0.037294		6 -1.397958 -1.335606 -0.120022
	6 -0.541280 -0.444615 0.034114		6 -0.421138 -0.358355 0.081398
	6 -0.700104 0.920667 -0.028290		1 -2.467670 2.361859 0.093451
	1 -1.959727 2.642802 -0.100914		1 -4.181060 0.593805 -0.257582
	1 -4.022386 1.249339 -0.103727		1 -3.462794 -1.763841 -0.390007
	1 -3.826165 -1.202631 -0.013318		1 -1.124201 -2.371498 -0.198341
	1 -1.645198 -2.290813 0.077907		7 0.944805 -0.716261 0.203769
	7 0.749045 -0.981814 0.071841		6 1.985988 0.067428 -0.238777
	6 1.831917 -0.145122 0.103671		8 3.075792 -0.404431 -0.477886
	8 2.958733 -0.537631 -0.091347		6 1.265335 -2.107824 0.481557
	6 0.948931 -2.406554 -0.100628		1 2.289284 -2.162328 0.816226
	1 2.009953 -2.599428 -0.098820		6 1.738423 1.514057 -0.393290
	6 1.552971 1.286319 0.437572		1 2.095654 1.957113 -1.306545
	6 2.119278 2.282413 -0.258742		6 -0.878440 0.940670 0.156274
	1 2.657539 2.088159 -1.170131		6 1.105917 2.229480 0.542765
	1 2.021419 3.305874 0.057095		1 0.936920 3.284842 0.412944
	1 1.107164 1.474352 1.400302		1 0.887180 1.823987 1.514296
	1 0.483141 -2.954411 0.711777		1 0.610010 -2.474785 1.260874
	1 0.527003 -2.741187 -1.043386		1 1.163503 -2.734527 -0.400569
TS20a	6 -1.469668 2.087806 1.101609	**TS21a**	6 -1.266464 1.576274 1.736034
	1 -0.600942 2.058457 1.755897		1 -0.238978 1.816401 1.998963
	1 -2.328128 2.270582 1.745602		1 -1.769773 1.317270 2.666125
	6 -3.437347 0.154382 -1.136516		6 -3.248292 -0.747361 -0.134464
	1 -3.242492 0.921624 -1.882488		1 -3.675312 0.113161 -0.644091
	1 -4.300075 0.493108 -0.565368		1 -3.840330 -0.896899 0.766817
	6 -2.112397 -1.346910 1.810883		6 -0.343288 -1.876178 1.600233
	1 -2.287847 -2.312089 1.341150		1 -0.230279 -2.712134 0.913863
	1 -3.047605 -1.064538 2.291277		1 -1.073409 -2.187415 2.345759
	6 -1.328447 3.219112 0.086879		6 -1.939682 2.782264 1.086912
	1 -2.202853 3.246115 -0.563121		1 -2.969832 2.538000 0.827317
	1 -0.478039 3.030693 -0.569151		1 -1.442748 3.025688 0.148908
	6 -3.748990 -1.174130 -1.819580		6 -3.330397 -1.982137 -1.027172
	1 -3.931495 -1.944570 -1.070422		1 -2.891629 -2.840677 -0.518527
	1 -2.883229 -1.511247 -2.389690		1 -2.733675 -1.830169 -1.926997
	6 -1.003314 -1.465487 2.851998		6 0.990852 -1.558748 2.269243
	1 -0.827106 -0.498049 3.322377		1 0.873898 -0.716384 2.951003
	1 -0.065381 -1.737153 2.367088		1 1.716920 -1.242867 1.521183

	6 -1.154889 4.591901 0.727859		6 -1.942617 4.021168 1.975970
	1 -0.279228 4.573809 1.375543		1 -0.915103 4.275456 2.232689
	1 -2.007058 4.790934 1.376145		1 -2.441869 3.785956 2.915257
	6 -1.015099 5.713624 -0.290876		6 -2.616668 5.219779 1.324434
	1 -1.892430 5.772399 -0.930456		1 -3.655776 5.003462 1.087771
	1 -0.894525 6.678208 0.193886		1 -2.600369 6.088269 1.976926
	1 -0.151330 5.555166 -0.932098		1 -2.118134 5.491104 0.397404
	6 -4.952357 -1.108777 -2.753722		6 -4.754310 -2.337035 -1.441523
	1 -4.772969 -0.346990 -3.511292		1 -5.197182 -1.484885 -1.955012
	1 -5.822699 -0.776818 -2.189236		1 -5.354462 -2.498378 -0.547102
	6 -5.257791 -2.437944 -3.428586		6 -4.827719 -3.566864 -2.334564
	1 -5.474547 -3.209577 -2.693771		1 -4.417938 -4.440256 -1.832758
	1 -6.116694 -2.360303 -4.089093		1 -5.852609 -3.796031 -2.611922
	1 -4.413323 -2.778400 -4.022938		1 -4.262591 -3.418984 -3.251707
	6 -1.301379 -2.490641 3.940785		6 1.571114 -2.736169 3.045342
	1 -1.471981 -3.460991 3.476699		1 1.702862 -3.577784 2.366544
	1 -2.233790 -2.222094 4.435574		1 0.849830 -3.059882 3.794789
	6 -0.189753 -2.606518 4.973381		6 2.896456 -2.411070 3.718525
	1 -0.018858 -1.656102 5.473370		1 2.785032 -1.593799 4.427217
	1 -0.430543 -3.342096 5.735518		1 3.287595 -3.267270 4.260973
	1 0.746363 -2.906585 4.508649		1 3.641716 -2.111925 2.985883
	50 -1.738768 0.105240 0.228059		0 -1.233074 -0.216832 0.502032
	1 -0.241126 -0.382880 -0.706742		1 -0.241223 0.143231 -1.024718
	6 1.083110 -0.989639 -1.569342		6 0.508550 0.477789 -2.414571
	6 2.200163 -1.078078 -0.574513		6 1.114209 1.757705 -2.090699
	1 0.637772 -1.927190 -1.861242		6 1.381759 -0.711693 -2.626380
	1 1.175156 -0.253176 -2.351451		1 -0.379034 0.571656 -3.015758
	6 2.978530 0.185599 -0.344819		7 2.375099 1.721338 -1.530144
	6 3.291975 -2.058815 -1.021364		8 0.529751 2.812334 -2.267382
	1 1.816456 -1.475449 0.366894		6 2.547674 -0.701490 -1.683771
	6 2.585690 1.439097 0.058136		1 1.747045 -0.712014 -3.657861
	6 4.319847 -0.063848 -0.621562		1 0.812225 -1.630342 -2.512859
	7 4.483473 -1.391400 -1.018254		6 3.008543 0.516678 -1.176265
	8 3.139137 -3.215755 -1.318018		6 3.192733 -1.871595 -1.325683
	6 3.544294 2.442342 0.186766		6 4.110275 0.522614 -0.324580
	1 1.551221 1.647775 0.270215		6 4.292186 -1.865622 -0.484546
	6 5.284445 0.913186 -0.500883		1 2.825751 -2.804911 -1.720834
	6 4.873298 2.177301 -0.089216		6 4.746099 -0.659318 0.012927
	1 3.248750 3.427602 0.502414		1 4.476283 1.445141 0.083749
	1 6.319006 0.713855 -0.717104		1 4.780974 -2.787233 -0.221551
	1 5.605482 2.959747 0.013120		1 5.596044 -0.628275 0.672760
	6 5.741147 -1.989912 -1.386096		6 2.998901 2.983273 -1.181159
	1 5.554621 -3.021495 -1.649033		1 2.451298 3.772827 -1.669695
	1 6.175521 -1.476631 -2.238764		1 2.976294 3.157536 -0.108450

	1 6.440541 -1.953701 -0.556307		1 4.029009 2.993341 -1.519041
TS47c	6 2.389830 1.304841 0.061524	**TS48c**	6 2.261589 1.409521 0.291228
	6 3.315907 0.263626 0.024153		6 3.264072 0.448818 0.168836
	6 2.865977 -1.041920 -0.066781		6 2.918820 -0.856525 -0.134469
	6 1.511446 -1.340765 -0.123348		6 1.595970 -1.233789 -0.321593
	6 0.576883 -0.308456 -0.101493		6 0.584704 -0.284210 -0.198773
	6 1.069353 0.973693 -0.016859		6 0.973355 0.997365 0.118521
	1 2.710634 2.330229 0.136665		1 2.499639 2.433487 0.525349
	1 4.370363 0.475160 0.066869		1 4.295462 0.720965 0.312388
	1 3.576388 -1.850215 -0.088644		1 3.688522 -1.602835 -0.229747
	1 1.199394 -2.368058 -0.176328		1 1.369018 -2.257964 -0.555649
	7 -0.807886 -0.501034 -0.171517		7 -0.778645 -0.557222 -0.366868
	6 -1.648619 0.566698 -0.013855		6 -1.683959 0.464845 -0.269940
	8 -2.834195 0.489255 -0.242086		8 -2.869448 0.260975 -0.143006
	6 -1.375955 -1.791646 -0.544013		6 -1.275492 -1.926905 -0.418486
	1 -2.290374 -1.588108 -1.083192		1 -2.263499 -1.880732 -0.853379
	6 -1.036098 1.833376 0.494627		6 -1.136630 1.852378 -0.374751
	6 -1.318826 3.016193 -0.069224		6 -1.567208 2.828241 0.437591
	1 -1.862091 3.075487 -0.996268		1 -2.195600 2.609880 1.283418
	1 -0.980554 3.936570 0.372745		1 -1.268758 3.850235 0.284939
	1 -0.583336 1.786656 1.471269		1 -0.593929 2.087974 -1.275159
	6 -1.664648 -2.678616 0.655450		1 -0.647010 -2.488035 -1.100497
	1 -2.077593 -3.626781 0.324269		6 -1.336061 -2.593669 0.945441
	1 -0.766376 -2.881549 1.229895		1 -1.703379 -3.610408 0.843318
	1 -2.388483 -2.205839 1.310840		1 -0.358586 -2.633116 1.415238
	1 -0.690715 -2.272501 -1.231908		1 -2.010740 -2.053114 1.600268
TS49c	6 -2.625963 0.976346 -0.090124	**TS50c**	6 -2.715957 1.034783 -0.504381
	6 -3.322320 -0.224809 -0.167418		6 -3.275758 -0.163083 -0.097261
	6 -2.615478 -1.411397 -0.095396		6 -2.435655 -1.195088 0.305066
	6 -1.236181 -1.422412 0.043594		6 -1.087524 -0.969146 0.289755
	6 -0.514649 -0.228330 0.125697		6 -0.477581 0.196401 -0.123953
	1 -3.144845 1.919202 -0.136414		6 -1.342330 1.218305 -0.523390
	1 -4.392861 -0.228865 -0.279113		1 -3.351218 1.844235 -0.820118
	1 -3.136593 -2.351228 -0.155497		1 -4.344028 -0.295103 -0.089279
	1 -0.733323 -2.370151 0.077793		1 -2.837954 -2.139676 0.630840
	7 0.895067 -0.234746 0.278718		7 0.931224 0.379147 -0.151181
	6 1.729235 0.781287 -0.120312		6 1.825885 -0.635035 -0.408148
	8 2.928015 0.616568 -0.195898		8 2.974766 -0.418879 -0.728236
	6 1.561919 -1.470931 0.697642		6 1.350935 -2.027465 -0.265860
	1 2.435993 -1.176928 1.262526		1 1.552646 -2.680251 -1.097332
	6 1.133537 2.092437 -0.450244		6 0.719019 -2.451588 0.832232
	1 1.422478 2.513678 -1.397566		1 0.392286 -3.473430 0.923613
	6 -1.268872 0.925527 0.061925		1 0.648240 -1.843554 1.716325
	6 0.285559 2.715314 0.373801		6 1.462101 1.744124 -0.142480

	1 -0.134542 3.672598 0.115984		1 2.519943 1.654892 -0.331701
	1 0.114875 2.371911 1.378406		1 -0.956240 2.163906 -0.854839
	1 0.894727 -1.985529 1.377454		6 1.224676 2.454524 1.178576
	6 1.986279 -2.373334 -0.450403		1 1.651653 3.452000 1.135954
	1 2.452791 -3.270650 -0.053957		1 0.169929 2.550655 1.412041
	1 1.145507 -2.674720 -1.066265		1 1.704586 1.916346 1.989937
	1 2.707810 -1.866833 -1.079770		1 1.046597 2.306604 -0.972225
TS59c	6 2.210234 1.667666 0.047636	**TS60c**	6 -3.127624 1.674960 0.717946
	6 3.089985 2.738899 0.185355		1 -2.591077 2.168941 1.524846
	6 4.438096 2.569928 -0.073313		1 -4.076549 1.344208 1.136559
	6 4.945495 1.338615 -0.475606		6 -3.158099 -1.277933 -1.273504
	6 4.058200 0.291361 -0.607043		1 -3.404868 -0.625631 -2.108306
	6 2.699204 0.444873 -0.345172		1 -4.102000 -1.537574 -0.797341
	1 1.160107 1.800163 0.243743		6 -1.616435 -1.309658 1.944574
	1 2.719321 3.700673 0.493983		1 -1.124967 -2.229668 1.635159
	1 5.110721 3.403235 0.036386		1 -2.583016 -1.603381 2.350354
	1 5.995358 1.218464 -0.674955		6 -3.370542 2.654687 -0.426533
	7 4.317909 -1.020836 -1.010444		1 -3.897701 2.155501 -1.239767
	6 3.175339 -1.768409 -1.023664		1 -2.417918 2.980884 -0.843860
	8 3.107144 -2.932374 -1.326342		6 -2.462036 -2.537133 -1.781378
	6 5.618963 -1.549939 -1.364665		1 -2.210791 -3.188487 -0.944030
	1 5.440292 -2.414137 -1.991841		1 -1.513868 -2.273848 -2.250405
	6 2.013982 -0.870177 -0.581456		6 -0.789170 -0.607252 3.017157
	6 0.895172 -0.860295 -1.577557		1 -1.282344 0.315443 3.323035
	1 0.518148 -1.826846 -1.870967		1 0.175277 -0.308649 2.605960
	1 0.934997 -0.118002 -2.358536		6 -4.168479 3.886332 -0.012526
	1 1.657383 -1.295913 0.358424		1 -3.645125 4.391915 0.797840
	6 6.451453 -1.939385 -0.154075		1 -5.126797 3.568360 0.396103
	1 7.416794 -2.319390 -0.474419		6 -4.399246 4.861379 -1.157674
	1 6.622082 -1.090902 0.500827		1 -4.949293 4.390261 -1.968829
	1 5.952866 -2.716133 0.416152		1 -4.967840 5.728126 -0.832951
	1 6.133514 -0.807081 -1.966703		1 -3.455876 5.218110 -1.563826
	1 -0.466089 -0.350209 -0.711289		6 -3.297242 -3.329952 -2.780814
	0 -1.987163 0.056079 0.224789		1 -3.548240 -2.685988 -3.622569
	6 -3.716835 -0.401048 -1.019808		1 -4.243105 -3.603360 -2.315107
	6 -2.067727 -1.125546 2.056209		6 -2.596359 -4.582081 -3.287071
	6 -1.997826 2.179871 0.728606		1 -2.363329 -5.258932 -2.468467
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	1 -3.673522 0.239650 -1.897751		1 -1.661730 -4.333660 -3.784202
	1 -4.604233 -0.102235 -0.464457		6 -0.545813 -1.463362 4.255202
	6 -0.920623 -0.877277 3.031188		1 -0.043249 -2.382691 3.957741
	1 -2.097244 -2.175543 1.773880		1 -1.505535 -1.762952 4.674106
	1 -3.020418 -0.909386 2.536480		6 0.276821 -0.753057 5.320244
	6 -1.919360 3.122404 -0.469181		1 -0.219175 0.153913 5.657561

	1 -1.172934 2.371193 1.411925 1 -2.909120 2.369261 1.293323 6 -5.052320 -2.154163 -2.304210 1 -3.863614 -2.503612 -0.560742 1 -2.935886 -2.160378 -1.991907 6 -1.004214 -1.726222 4.295019 1 -0.894993 0.173964 3.318146 1 0.033220 -1.075767 2.541720 6 -1.941994 4.597782 -0.084151 1 -2.747806 2.927816 -1.150262 1 -1.012381 2.925220 -1.041150 6 -5.158234 -3.614517 -2.718308 1 -5.019088 -1.523905 -3.191955 1 -5.948849 -1.863074 -1.758437 6 0.145082 -1.476401 5.260512 1 -1.024118 -2.778356 4.014469 1 -1.951324 -1.527041 4.794678 6 -1.861496 5.529663 -1.284416 1 -1.113416 4.801055 0.593138 1 -2.851245 4.803980 0.478776 1 -4.286881 -3.923554 -3.290582 1 -5.227473 -4.264090 -1.849050 1 -6.036511 -3.790588 -3.332837 1 1.102348 -1.700805 4.796189 1 0.170116 -0.437058 5.579282 1 0.057280 -2.092855 6.150570 1 -0.945839 5.364844 -1.847188 1 -2.696780 5.368420 -1.961604 1 -1.879479 6.572322 -0.980250		1 0.433878 -1.386164 6.188846 1 1.253902 -0.470304 4.936137 0 -2.006738 -0.109604 0.162766 1 -0.426172 0.400225 -0.611490 6 0.984246 1.023595 -1.307447 6 2.019080 0.954453 -0.226191 1 1.107042 0.364830 -2.152123 1 0.604156 2.006780 -1.533790 6 2.717645 -0.365144 -0.067387 6 3.188103 1.913727 -0.479833 1 1.577066 1.276201 0.718779 6 2.231664 -1.628298 0.171188 6 4.088458 -0.162101 -0.203269 7 4.345925 1.190447 -0.441164 8 3.113735 3.100828 -0.670034 6 3.125452 -2.691139 0.279978 1 1.173614 -1.797637 0.273343 6 4.989648 -1.200498 -0.098385 6 5.655664 1.774135 -0.646498 6 4.484801 -2.473257 0.148122 1 2.756867 -3.684492 0.467198 1 6.047988 -1.043565 -0.206189 1 5.562193 2.828331 -0.418557 1 5.168299 -3.300546 0.233452 1 6.336592 1.340108 0.079470 6 6.177334 1.584587 -2.061589 1 7.160946 2.034467 -2.156901 1 6.259993 0.533322 -2.318337 1 5.515466 2.059930 -2.777868
TS61c	6 -1.647255 1.761769 1.633847 1 -0.682663 1.952156 2.098557 1 -2.350504 1.580885 2.445101 6 -3.412505 -0.653529 -0.337322 1 -3.784837 0.189229 -0.915048 1 -4.100667 -0.783757 0.496149 6 -0.728698 -1.696807 1.766219 1 -0.615553 -2.584277 1.148016 1 -1.512108 -1.921984 2.488199 6 -2.083763 2.972916 0.814239 1 -3.050335 2.779222 0.348652 1 -1.383899 3.139909 -0.003177 6 -3.388143 -1.912496 -1.199115 1 -3.002948 -2.752993 -0.621567 1 -2.696156 -1.779289 -2.031092		

	6 0.579806 -1.387221 2.487071 1 0.468373 -0.486751 3.091320 1 1.361287 -1.169315 1.760247 6 -2.188197 4.251728 1.638198 1 -1.223634 4.453734 2.102040 1 -2.891995 4.094623 2.454789 6 -2.619893 5.456363 0.814710 1 -3.596412 5.293176 0.364883 1 -2.682916 6.353074 1.424793 1 -1.915629 5.650745 0.009893 6 -4.755050 -2.291599 -1.758666 1 -5.144777 -1.456910 -2.339578 1 -5.448963 -2.436639 -0.931930 6 -4.720547 -3.543712 -2.622591 1 -4.363047 -4.400566 -2.056501 1 -5.706669 -3.789504 -3.005959 1 -4.058047 -3.412857 -3.474914 6 1.054113 -2.521810 3.388886 1 1.181324 -3.421610 2.788675 1 0.275815 -2.747983 4.116755 6 2.353929 -2.203588 4.113135 1 2.244628 -1.325732 4.745680 1 2.669070 -3.028763 4.745663 1 3.154062 -2.002397 3.405398 0 -1.481394 -0.090130 0.501207 1 -0.325541 0.198726 -0.921951 6 0.568118 0.436989 -2.243914 6 1.397667 1.549632 -1.817044 6 1.191538 -0.895641 -2.472232 1 -0.237202 0.737840 -2.891332 7 2.568004 1.240804 -1.151802 8 1.057597 2.706574 -1.997674 6 2.290915 -1.159176 -1.487501 1 1.596819 -0.935010 -3.487824 1 0.443169 -1.682707 -2.422257 6 2.955455 -0.087359 -0.882551 6 2.676828 -2.455090 -1.191623 6 4.011328 -0.360660 -0.014291 6 3.720126 -2.723296 -0.324213 1 2.147532 -3.268644 -1.660482 6 4.387432 -1.663210 0.258673 1 4.553159 0.436539 0.455523 1 4.005776 -3.738396 -0.111240 1 5.206755 -1.840970 0.933910		

	6 3.384614 2.357014 -0.684812 1 2.750687 3.229386 -0.718717 1 3.647755 2.193882 0.354002 6 4.622304 2.584989 -1.536650 1 5.194233 3.419689 -1.141807 1 5.267773 1.712972 -1.557089 1 4.338465 2.822289 -2.556828		
TS52d	6 2.717364 0.870791 0.217204 6 3.387361 -0.338561 0.049337 6 2.654046 -1.490061 -0.177458 6 1.267748 -1.470069 -0.239399 6 0.579276 -0.273010 -0.051743 6 1.354440 0.841178 0.180505 1 3.256647 1.788215 0.382792 1 4.462261 -0.374564 0.091680 1 3.163892 -2.427369 -0.319102 1 0.744472 -2.384701 -0.436924 7 -0.817710 -0.125242 -0.087192 6 -1.333047 1.148552 -0.116588 8 -2.500399 1.384357 0.096733 6 -1.762882 -1.238505 0.120167 1 -2.704611 -0.733810 0.277295 6 -0.386127 2.251042 -0.466400 6 -1.926020 -2.102771 -1.124982 1 -2.750361 -2.793356 -0.973754 1 -2.160396 -1.485467 -1.986076 1 -1.045752 -2.689917 -1.360018 6 -0.453195 3.437448 0.151908 1 -1.082728 3.579886 1.012865 1 0.143799 4.269443 -0.177198 1 0.171466 2.141898 -1.381207 6 -1.470175 -2.033005 1.385941 1 -2.294970 -2.714433 1.570236 1 -0.563180 -2.622438 1.324226 1 -1.386103 -1.369718 2.240718	**TS53d**	6 2.849125 0.746955 0.250198 6 3.524376 -0.462024 0.098967 6 2.798601 -1.612840 -0.152628 6 1.414123 -1.594105 -0.254458 6 0.721058 -0.396735 -0.084704 6 1.488127 0.718028 0.172441 1 3.383270 1.663721 0.435094 1 4.597462 -0.498085 0.173860 1 3.312748 -2.549487 -0.282427 1 0.901990 -2.512466 -0.474369 7 -0.675240 -0.246724 -0.165847 6 -1.186209 1.025308 -0.146058 8 -2.348618 1.253589 0.096789 6 -1.574345 -1.402700 0.021669 1 -0.948061 -2.271570 -0.114114 6 -0.238193 2.132434 -0.480530 6 -2.131697 -1.463373 1.438728 1 -2.680980 -2.390880 1.572245 1 -1.327673 -1.441174 2.168321 1 -2.800560 -0.634463 1.630326 6 -0.313743 3.313249 0.149177 1 -0.950021 3.443679 1.007106 1 0.281906 4.151085 -0.167334 1 0.324551 2.034924 -1.393554 6 -2.653654 -1.469870 -1.049436 1 -3.186026 -2.411859 -0.956552 1 -3.365819 -0.661713 -0.951368 1 -2.212582 -1.429306 -2.040820
TS54d	6 -2.851951 0.626880 0.243526 6 -3.342935 -0.594145 -0.203325 6 -2.448460 -1.584205 -0.570466 6 -1.080155 -1.377333 -0.498772 6 -0.561516 -0.168980 -0.031588 1 -3.521667 1.421794 0.525688 1 -4.404148 -0.762557 -0.269731 1 -2.813187 -2.529446 -0.933693 1 -0.422217 -2.160343 -0.821287	**TS55d**	6 -2.971771 0.625939 0.249321 6 -3.494817 -0.636045 -0.007305 6 -2.625908 -1.685978 -0.247314 6 -1.252739 -1.499539 -0.236216 6 -0.702332 -0.244255 0.035241 1 -3.620472 1.465198 0.436308 1 -4.559895 -0.791436 -0.022623 1 -3.014923 -2.666684 -0.460275 1 -0.617778 -2.337792 -0.456319

	7 0.840474 0.060767 0.047895		7 0.707219 -0.046827 0.053699
	6 1.408844 1.255827 -0.320067		6 1.299116 1.086784 -0.447937
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	1 2.120784 -2.502833 1.883811		1 2.669715 -2.804370 -0.501970
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	1 1.508124 -2.480571 -1.216081		1 3.373908 -0.167528 1.032505
	1 2.610453 -1.161485 -1.600358		1 2.156389 -0.340942 2.296669
TS68d	6 -2.275719 2.154458 0.633284	**TS69d**	6 -2.290114 2.115836 0.696418
	1 -1.475407 2.385319 1.333273		1 -1.510910 2.332884 1.427943
	1 -3.207072 2.333557 1.167831		1 -3.241103 2.290478 1.201708
	6 -3.833558 -0.480106 -1.169419		6 -3.817161 -0.494590 -1.178517
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	1 -2.956284 -2.222318 -2.089789		1 -2.900435 -2.213690 -2.120506
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	1 -3.191782 4.745984 0.289821		1 -3.186094 4.721637 0.378013
	6 -2.179940 5.450625 -1.469248		6 -2.110317 5.465915 -1.334246
	1 -2.993413 5.245979 -2.161091		1 -2.901958 5.279800 -2.057608
	1 -2.235205 6.500430 -1.195725		1 -2.170346 6.510442 -1.038452
	1 -1.246459 5.297063 -2.005321		1 -1.158780 5.318312 -1.841697

	6 -5.048271 -2.259679 -2.534405		6 -4.993612 -2.271162 -2.592607
	1 -4.971985 -1.628413 -3.418758		1 -4.913809 -1.621747 -3.465252
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	6 -5.097587 -3.721658 -2.953331		6 -5.017806 -3.730887 -3.038203
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	1 -0.402280 -0.311659 5.675374		1 -0.194541 -0.574121 5.599810
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	1 0.888980 -0.191517 -2.201227		1 0.909819 -0.155909 -2.179515
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	6 3.076626 -1.700746 -0.627673		6 3.198519 -1.482835 -0.573107
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	6 1.958293 1.757256 0.160449		6 1.847092 1.918825 0.146099
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	7 4.207341 -0.929993 -0.592176		7 4.278617 -0.633013 -0.554617
	8 3.042483 -2.883490 -0.855380		8 3.240312 -2.694660 -0.792264
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TS70d	6 -1.168608 1.754768 1.729612	**TS71d**	6 -1.157540 1.825404 1.785508
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	1 -2.102622 -1.963886 2.159825		1 -2.159265 -1.808638 2.322064
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