Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supplementary Materials for Surface Hopping Simulations for Deactivation Pathways of a PLATICT System

Julia Haberhauer[1]*, Sebastian Mai[2], Leticia González[2] and Christof Hättig[1]

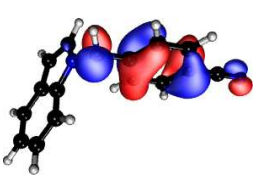
[1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum 44780, Germany.

[2]Institut für Theoretische Chemie, Universität Wien, Wien 1090, Österreich.

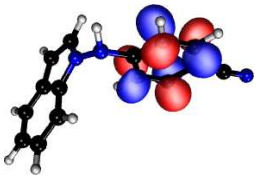
*Corresponding author. Email: julia.haberhauer@rub.de

Contents

1 NTOs of ground and excited state minima

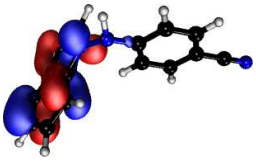


(occ.)

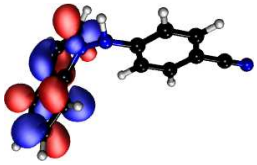


(vir.)

(a) S_1 (4.67 eV, 0.015 osc)

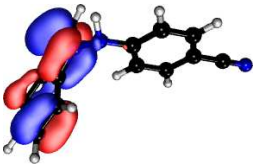


(occ.)

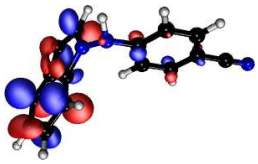


(vir.)

(b) S_2 (4.71 eV, 0.065 osc)

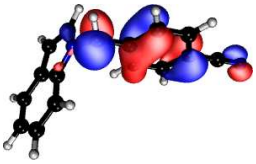


(occ.)

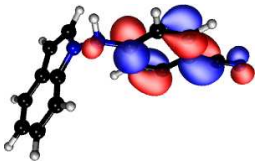


(vir.)

(c) S_3 (4.99 eV, 0.226 osc)

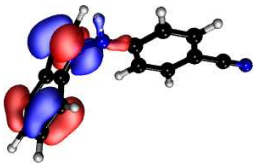


(occ.)

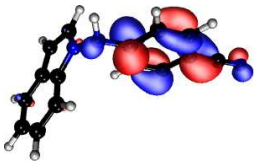


(vir.)

(d) S_4 (5.13 eV, 0.414 osc)



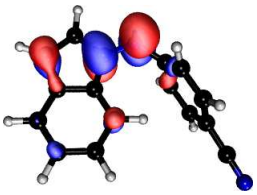
(occ.)



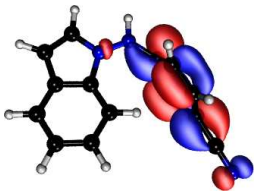
(vir.)

(e) S_5 (5.21 eV, 0.073 osc)

Figure S1 Vertical transitions obtained with ADC(2)/aug-cc-pVTZ in vacuum at the ground-state minimum S_0-Min-2 (structure optimized at the MP2/aug-cc-pVTZ level). For each state the most important occupied and virtual NTO is shown.



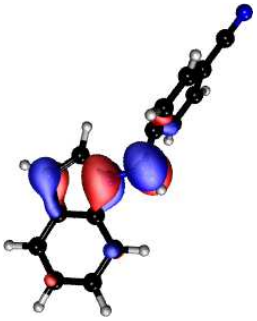
(occ.)



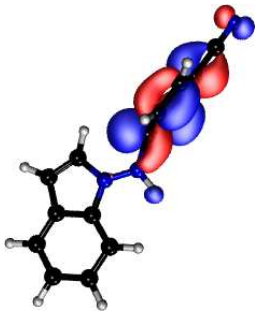
(vir.)

(a) S_1 (2.04 eV, 0.000 osc)

Figure S2 Electronic transitions of the S_1-Min-a, calculated using ADC(2)/cc-pVDZ in vacuum. Previous geometry optimization using ADC(2)/cc-pVDZ in vacuum. The most important occupied and virtual NTO of the transition is shown.



(occ.)



(vir.)

(a) S_1 (1.92 eV, 0.000 osc)

Figure S3 Electronic transitions of the S_1-Min-c, calculated using ADC(2)/aug-cc-pVTZ in vacuum. Previous geometry optimization using ADC(2)/aug-cc-pVTZ in vacuum. The most important occupied and virtual NTO of the transition is shown.

(occ.) (vir.)

(a) S_1 (1.74 eV, 0.000 osc)

Figure S4 Electronic transitions of the S_1-Min-d, calculated using ADC(2)/aug-cc-pVTZ in vacuum. Previous geometry optimization using ADC(2)/aug-cc-pVTZ in vacuum. The most important occupied and virtual NTO of the transition is shown.

2 Basis set comparison

Table S1 Vertical excitation energies and oscillator strengths at the ground state minimum S_0-Min-1 for different basis sets and methods. The structure was optimized with MP2/cc-pVDZ.

		S_1		S_2		S_3		S_4		S_5	
Basis Set	Method	eV	osc	eV	osc	eV	osc	eV	osc	eV	osc
cc-pVDZ	ADC(2)	4.78	0.005	4.80	0.058	5.14	0.195	5.25	0.234	5.34	0.222
	CC2	4.79	0.006	4.82	0.047	5.16	0.158	5.32	0.191	5.42	0.305
cc-pVTZ	ADC(2)	4.67	0.004	4.69	0.059	4.99	0.171	5.09	0.165	5.19	0.300
	CC2	4.68	0.005	4.71	0.047	5.01	0.140	5.15	0.134	5.26	0.358
aug-cc-pVDZ	ADC(2)	4.62	0.008	4.63	0.064	4.90	0.102	4.98	0.156	5.09	0.249
	CC2	4.64	0.000	4.66	0.060	4.90	0.094	5.01	0.114	5.13	0.080
aug-cc-pVTZ	ADC(2)	4.61	0.001	4.62	0.065	4.89	0.131	4.98	0.169	5.09	0.313
	CC2	4.62	0.002	4.64	0.054	4.89	0.112	5.02	0.129	5.15	0.342
SVP	ADC(2)	4.78	0.007	4.81	0.052	5.20	0.246	5.31	0.299	5.40	0.121
	CC2	4.80	0.007	4.84	0.043	5.23	0.188	5.39	0.282	5.47	0.197
TZVP	ADC(2)	4.66	0.003	4.68	0.061	4.97	0.165	5.06	0.168	5.16	0.302
	CC2	4.67	0.005	4.70	0.049	4.98	0.136	5.11	0.135	5.23	0.360

3 NTOs of the constituting aminoindole and dimethylaminobenzonitrile subsystems

(occ.) (vir.)

(a) S_1 (4.64 eV, 0.059 osc)

(occ.) (vir.)

(b) S_2 (4.90 eV, 0.097 osc)

Figure S5 Electronic transitions of aminoindole, calculated using ADC(2)/aug-cc-pVTZ in vacuum. Previous geometry optimization using MP2/aug-cc-pVTZ in vacuum. The most important occupied and virtual NTO of the transition is shown.

(occ.) (vir.)

(a) S_1 LE (2.96 eV, 0.054 osc)

(occ.) (vir.)

(b) S_1 PLICT (2.94 eV, 0.054 osc)

Figure S6 Electronic transitions of the locally excited (LE) and planarized intramolecular charge transfer (PLICT) S_1 minima of aminoindole, calculated using ADC(2)/aug-cc-pVTZ in vacuum. Previous geometry optimization using ADC(2)/aug-cc-pVTZ in vacuum. The most important occupied and virtual NTO of the transition is shown.

(occ.) (vir.)

(a) S_1 (4.38 eV, 0.028 osc)

(occ.) (vir.)

(b) S_2 (4.60 eV, 0.478 osc)

Figure S7 Electronic transitions of dimethylaminobenzonitrile, calculated using ADC(2)/aug-cc-pVTZ in vacuum. Previous geometry optimization using MP2/aug-cc-pVTZ in vacuum. The most important occupied and virtual NTO of the transition is shown.

(occ.) (vir.)

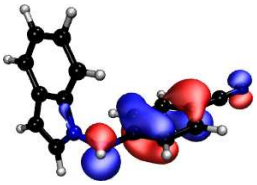
(a) S_1 LE (3.73 eV, 0.030 osc)

(occ.) (vir.)

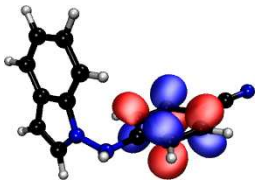
(b) S_1 TICT (2.45 eV, 0.001 osc)

Figure S8 Electronic transitions of the locally excited (LE) and twisted intramolecular charge transfer (TICT) S_1 minima of dimethylaminobenzonitrile, calculated using ADC(2)/aug-cc-pVTZ in vacuum. Previous geometry optimization using ADC(2)/aug-cc-pVTZ in vacuum. The most important occupied and virtual NTO of the transition is shown.

4 Solvation Effect

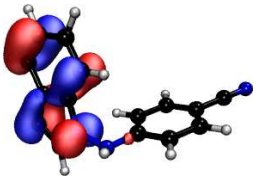


(occ.)

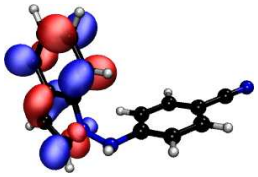


(vir.)

(a) S_1 (4.68 eV, 0.018 osc)

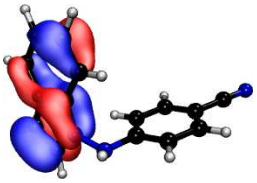


(occ.)

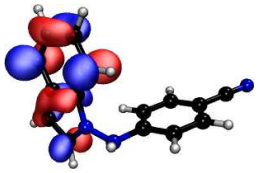


(vir.)

(b) S_2 (4.69 eV, 0.112 osc)

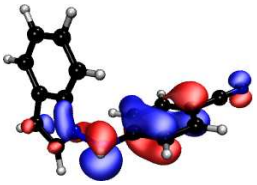


(occ.)

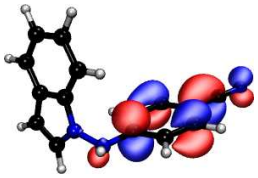


(vir.)

(c) S_3 (4.87 eV, 0.253 osc)

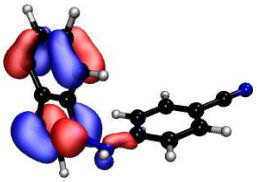


(occ.)

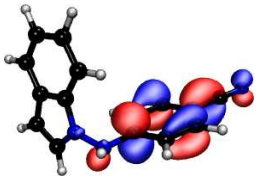


(vir.)

(d) S_4 (4.91 eV, 0.508 osc)



(occ.)



(vir.)

(e) S_5 (5.12 eV, 0.017 osc)

Figure S9 Vertical transitions obtained with COSMO-CC2/aug-cc-pVTZ in 1-chlorbutan at the ground-state minimum S_0-Min-1 (structure optimized at the COSMO-CC2/aug-cc-pVTZ level in 1-chlorbutan). For each state the most important occupied and virtual NTO is shown.

(occ.) (vir.)

(a) S_1 (4.69 eV, 0.112 osc)

(occ.) (vir.)

(b) S_2 (4.71 eV, 0.025 osc)

(occ.) (vir.)

(c) S_3 (4.88 eV, 0.342 osc)

(occ.) (vir.)

(d) S_4 (4.90 eV, 0.370 osc)

(occ.) (vir.)

(e) S_5 (5.10 eV, 0.021 osc)

Figure S10 Vertical transitions obtained with COSMO-ADC(2)/aug-cc-pVTZ in 1-chlorbutan at the ground-state minimum S_0-Min-1 (structure optimized at the COSMO-MP2/aug-cc-pVTZ level in 1-chlorbutan). For each state the most important occupied and virtual NTO is shown.

5 Diagnostics of Excited State Trajectories

In the final analysis, trajectories with problems in total energy conservation along the full trajectory (0.2 eV), energy smoothness between two time steps (0.1 eV for total energy, 0.7 eV for kinetic energy, 0.7 eV for potential energy), maximum drift in total population (1.0^{-07}), hopping energy restriction (1 eV), or intruder states were excluded.

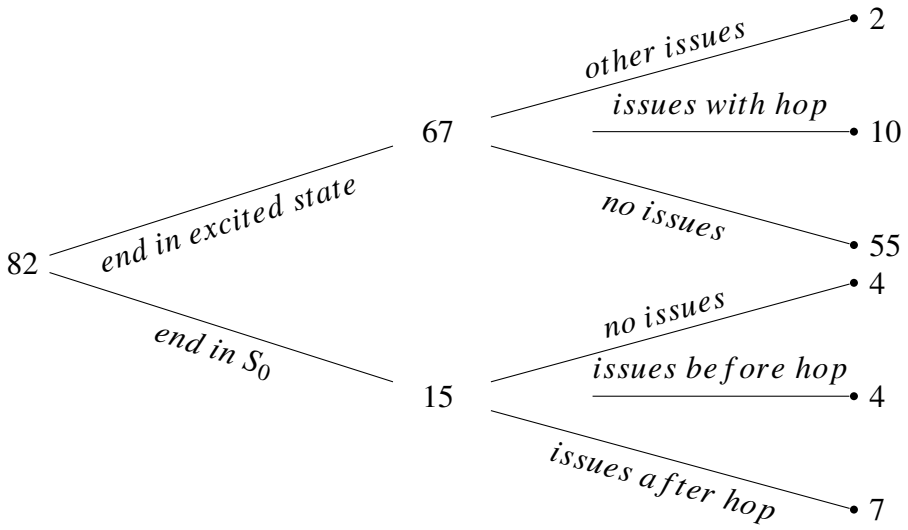


Figure S11 Tree diagram of the excited state trajectories. Shown are which trajectories terminate with and without issues in the excited state and in the ground state. Trajectories with problems in energy conservation, potential or kinetic energy smoothness, hopping energy restriction, or intruder states were excluded as in the default settings of SHARC's diagnostic tool.

6 Distribution of Ground State minima

Table S2 Distributions of the end structure (S_0-Min-1 and its enantiomer E-S_0-Min-1 or S_0-Min-2 and its enantiomer E-S_0-Min-2) in percent depending on the excited state minimum the trajectories were started from.

	S_1-Min-a	S_1-Min-b	S_1-Min-c	S_1-Min-d
S_0-Min-1	29	9	43	38
E-S_0-Min-1	20	4	38	56
S_0-Min-2	31	45	5	6
E-S_0-Min-2	20	42	14	0

7 Coordinates of S_0 and S_1 minima

We shall briefly discuss how the following minima of S_0 and S_1 have been identified. For the S_0 minima due to the rigidity of the molecule with only the two torsional angles (that are pointed out in the manuscript) as flexible degrees of freedom, only two symmetry-distinct ground state minima (plus their enantiomers) are expected. This has been confirmed by a calculation with the conformer-Rotamer Ensemble Sampling Tool (CREST). For the excited state minima, we first optimized from the Franck-Condon point of the ground state minima. In addition, we started geometry optimizations from different potential excited-state structures such as PLICT or TICT structures. Furthermore, we performed relaxed PES scans along the flexible dihedrals for the LE, PLICT, TICT, and PLATICT structures. Also, after the excited state dynamics we optimized all final structures. We distinguish the minima that were reached by the trajectories after geometry optimization by their visual match and specifically the agreement of the angles d_1 and d_2 within about 2°.

Table S3 Cartesian coordinates in a.u. of the optimized ground state minimum S_0-Min-1 at MP2/aug-cc-pVTZ level of theory.

−5.07419860188774	−0.46209032629199	−1.23167331868437	c
−3.08634477960059	−0.28117013994855	0.56087510172389	c
−2.53819709872613	1.92479289969882	1.89878838625082	c
−4.08006959690107	3.99657568249328	1.44113178664853	c
−6.09505133363682	3.86196652736228	−0.29682086082858	c
−6.60768492487058	1.66769898350683	−1.63395600468579	c
−0.97523368419556	2.02353735752560	3.21677897098778	h
−3.72373261958017	5.75079083787670	2.42999818028430	h
−7.25726192829138	5.51806320633184	−0.59541506056205	h
−8.15493103154670	1.59918050009391	−2.97164265867005	h
−1.91706550623592	−2.60616894736571	0.62659176060526	n
−3.02833024731727	−4.20455547156977	−1.10477635407386	c
−4.99480360115417	−2.95887683536675	−2.26065872500554	c
−2.30756325081487	−6.09696899603363	−1.32122498651698	h
−6.23877139467335	−3.75457862420495	−3.66298010168496	h
0.30870234134104	−3.15176534253963	1.87447129643560	n
0.06079002166623	−3.14600180112724	3.77399507846903	h
2.43322811204012	−1.76443390676789	1.06712703403430	c
4.51019024548208	−1.53200604648348	2.68126968540025	c
2.52143865695914	−0.72105154109904	−1.35632229694416	c
6.66585454239182	−0.26895300576436	1.88750008589178	c
4.43794081309258	−2.34706368608967	4.55886800182831	h
4.67865393548838	0.54341442399719	−2.15447143589595	c
0.90805307266393	−0.89551450661109	−2.60238883504339	h
8.27337027459403	−0.08333240630435	3.13659300617037	h
4.75252554086596	1.36047929494041	−4.02693425827619	h
6.75952446330422	0.77802043757222	−0.54059979427790	c
8.97387753711041	2.08788832641372	−1.36187758700353	c
10.79509004243225	3.16212329472789	−2.03224609657699	n

Table S4 Cartesian coordinates in a.u. of the optimized ground state minimum S_0-Min-2 at MP2/aug-cc-pVTZ level of theory.

−5.62824879245359	−0.21652573799773	−1.43179867550567	c
−4.08866098437178	0.09933806101256	0.74193280723193	c
−4.29911183859114	2.15580220287537	2.37847094141696	c
−6.14977782819480	3.92485064549174	1.81396096147621	c
−7.73506149298159	3.64326296145088	−0.31046106754983	c
−7.49777376005774	1.60173922193958	−1.93396520796241	c
−3.06950803164361	2.34531042669243	4.00127273715114	h
−6.38352925602148	5.55415967464369	3.02784626773920	h
−9.16094456755369	5.06252009880822	−0.67825320577543	h
−8.72059122594755	1.41579011145933	−3.56433906104803	h
−2.46120869838470	−1.92754338712694	0.81965343209597	n
−2.84235783685786	−3.44387782393875	−1.27465111683588	c
−4.80833305876069	−2.47351333251535	−2.66917141987763	c
−1.68052050421676	−5.09455964043812	−1.55895376638643	h
−5.57816855275573	−3.30039373845209	−4.36417186416624	h
−0.42208427444001	−2.03619177951465	2.43934771404231	n
−0.41074207795702	−3.64139957281795	3.47845266977450	h
1.92418589612107	−1.35213646655969	1.39909530540984	c
4.14733985677370	−2.08961347042866	2.62076957606625	c
2.04481555725231	0.15744761573624	−0.76487739939677	c
6.47825096749184	−1.33286682061571	1.69139955706861	c
4.04832871629269	−3.25246317326581	4.30360086603872	h
4.37877059068498	0.91932707729911	−1.69427061021197	c
0.32198960047680	0.73189988210975	−1.70745501341560	h
8.20050445556739	−1.90940651530799	2.62969556148571	h
4.48095530231968	2.08684597050698	−3.36938430095273	h
6.60527386383848	0.17945550122341	−0.47622279367909	c
9.00454009318469	0.95705310389959	−1.44182777884974	c
10.97752072969910	1.59215803234438	−2.23189094455051	n

Table S5 Cartesian coordinates in a.u. of the optimized ground state minimum S_1-Min-b at ADC(2)/aug-cc-pVTZ level of theory.

−5.08897210915896	−0.38566465718475	−0.07405976900825	c
−2.41515749100375	−0.50958013281045	−0.06208547782380	c
−0.88540011575923	1.62032979914128	0.11807269262886	c
−2.14200864965759	3.93709925887174	0.29018900274545	c
−4.78011047858545	4.10405651047226	0.28160171468106	c
−6.28609921735228	1.94966406180710	0.09978498777072	c
1.15167459619914	1.54878413750561	0.12925159429465	h
−1.01727682918792	5.63763473568026	0.43347689838065	h
−5.66597619080278	5.94158376128347	0.41882784867727	h
−8.32680567813253	2.08323077585567	0.09361911051547	h
−1.83063959870603	−3.10926604420314	−0.26188500719817	n
−4.06385990984228	−4.53404335979821	−0.39208152236126	c
−6.06015231823557	−2.92213791562663	−0.28133703056694	c
−3.94985261421319	−6.56277815375324	−0.55099018054291	h
−8.02233049236137	−3.46977321826572	−0.34037213948874	h
0.44422365563252	−4.16117659727488	−0.32624106476162	n
0.35631068107451	−6.07481644794557	−0.47764425928317	h
2.76064825561001	−2.77805760876919	−0.19889757937842	c
3.51691437269216	−1.84480024041068	2.23200479991966	c
3.55428108031048	−1.47698025881063	−2.44156882900601	c
5.09291973505179	0.20511751451637	2.39481605505659	c
2.86728536978858	−2.79684391280845	3.92882623806525	h
5.13003848514904	0.57126495673100	−2.25664622203250	c
2.93287379624698	−2.15107014533833	−4.27653768888222	h
5.73491157401141	0.86130454927586	4.22608493627431	h
5.80012979336097	1.50509965047569	−3.95228934012606	h
5.91009205177235	1.51801433508644	0.16439344968465	c
7.43845394537422	3.68491627706231	0.34718169376235	c
8.70855610739462	5.52285169332383	0.50206467396843	n

Table S6 Cartesian coordinates in a.u. of the optimized ground state minimum S_1-Min-c at ADC(2)/aug-cc-pVTZ level of theory.

−5.79498408862027	−0.71216162123814	−0.92513983164700	c
−4.05137133666772	0.23137836626328	0.85486366046326	c
−4.73380851560896	1.30308852532968	3.14205587425415	c
−7.32157051134285	1.42284502847381	3.64825660893960	c
−9.09735444038283	0.50112068537454	1.91666393856180	c
−8.36679566284579	−0.57153003896380	−0.37763356856626	c
−3.37298664384191	2.01992732665364	4.49058200153883	h
−7.95642854193544	2.24243086982925	5.40888456441708	h
−11.08529499104611	0.62659791233916	2.37512483279201	h
−9.76227545043772	−1.27532058084837	−1.69611567763643	h
−1.64119008648289	−0.16221915796069	−0.19909918234995	n
−1.85408829490576	−1.31876855588464	−2.57249678821411	c
−4.36280775479197	−1.66701397194263	−3.04454016546545	c
−0.14118593686282	−1.73009511106258	−3.59394099621966	h
−5.12348360569714	−2.51838917217483	−4.73191777033814	h
0.52139828930174	0.45545035175249	0.86501545158034	n
0.31499794961224	1.28524989211463	2.60287261468150	h
2.90177895219793	−0.01800697779813	−0.35119848281799	c
4.38435776868695	−2.03794179922855	0.69891745970459	c
4.18319908621759	2.16758262967848	−1.33212366087290	c
6.95434957292847	−2.06297348000435	0.35700582430882	c
3.44886018836960	−3.58309316917944	1.66995892082558	h
6.75454406118606	2.11477707560044	−1.66058004327600	c
3.09519734182784	3.81031265487745	−1.90074324881632	h
8.05903771585255	−3.64703425623600	1.03812587121680	h
7.70704455324318	3.71293785953453	−2.51623020164071	h
8.21186993875824	−0.03025267506830	−0.90247652201927	c
10.84774350048486	−0.08277564792871	−1.27211783603338	c
13.06185632847563	−0.12968476877686	−1.58820166022243	n

Table S7 Cartesian coordinates in a.u. of the optimized ground state minimum S_1-Min-d at ADC(2)/aug-cc-pVTZ level of theory.

−4.61242004855020	−1.75134070954659	−0.12128112126244	c
−3.76633961904776	0.63608022901372	0.70181584239758	c
−5.33698589888804	2.50618829846726	1.63451728781266	c
−7.91063953701010	1.92325131141670	1.73876825453376	c
−8.80849945406148	−0.43120398428027	0.93541840956374	c
−7.18590267167542	−2.28922946142227	0.00076681919788	c
−4.65659401148843	4.33211259623386	2.25966146979923	h
−9.22291400385892	3.31749322097033	2.45204347912823	h
−10.81302194330882	−0.81597557301411	1.04371473544368	h
−7.91176171198833	−4.09985719247605	−0.61235337057241	h
−1.12671025108619	0.63833407998071	0.36208772197660	n
−0.32387393357489	−1.67875846303138	−0.64643997974331	c
−2.41918038223028	−3.15084611939803	−0.95083850299026	c
1.65837858051280	−1.97779342587314	−1.01890466172971	h
−2.40425054020752	−5.04804891315943	−1.69336534470569	h
0.40903674513506	2.52784013262506	0.90102816152761	n
−0.47245975715935	4.07037661926957	1.62228715749291	h
3.10163168094173	2.31270784331563	0.47355444353954	c
4.38214354776713	0.61347247731584	2.17473099956017	c
3.83015947931587	2.30312422285813	−2.15128499283431	c
6.42258579025641	−0.75980714816181	1.36285730857201	c
3.75977862948363	0.48673077900800	4.12563939460099	h
5.87388582940103	0.91973239045422	−2.93731821412289	c
2.78818486545078	3.46011706436517	−3.48733764569261	h
7.44731084582261	−1.94425179254086	2.68355221012034	h
6.48065572773457	1.01444997959327	−4.89181617171958	h
7.24281438644529	−0.65757737702021	−1.21492748413312	c
9.30858095332156	−2.11235367416135	−2.04665360723615	c
11.03883639753445	−3.34605785251249	−2.74923516993218	n

Table S8 Cartesian coordinates in a.u. of the optimized ground state minimum S_0-Min-1 at MP2/cc-pVDZ level of theory.

−5.15908673089008	−0.46403943738307	−1.21740495180766	c
−3.10743605672376	−0.26556978776437	0.53106947128945	c
−2.55484722585500	1.96229703781701	1.87721106245296	c
−4.15112885688244	4.03003358506325	1.47129257656184	c
−6.22106334957809	3.87894047093171	−0.23259858911524	c
−6.74181567872282	1.66446524423661	−1.57467545616733	c
−0.94670691538512	2.07713486603792	3.17449453369660	h
−3.78946920154111	5.80231919866526	2.47609625812902	h
−7.42755195658922	5.53911803147624	−0.49715966083928	h
−8.33966920485873	1.57552333221392	−2.88798417671476	h
−1.90570125036900	−2.59277539369922	0.55777755189965	n
−3.06444707987819	−4.21488439148593	−1.14413310057966	c
−5.08862040116111	−2.97911442275899	−2.25668542202197	c
−2.32983752615533	−6.12585481068814	−1.37183690428258	h
−6.37944683049538	−3.79217677533164	−3.64107577305765	h
0.31978998595660	−3.17356051966140	1.81294152143477	n
0.05053144434942	−3.10667261462371	3.72620111433187	h
2.46518465738709	−1.76418118796090	1.03146876671618	c
4.52332020433740	−1.50439749300250	2.70085807065076	c
2.62215692452737	−0.76061079633129	−1.42960780451824	c
6.72007805376558	−0.24967867380071	1.93186302777258	c
4.40444170617010	−2.29311741391477	4.61261852920419	h
4.81729176510766	0.49931624311787	−2.20186714498040	c
1.02595301680716	−0.95990780673233	−2.72860470354996	h
8.31293664652538	−0.04361922839538	3.23391115069789	h
4.93762926234085	1.29007493777686	−4.10858374542643	h
6.87812281587903	0.76337880576121	−0.53056101358563	c
9.13461583807881	2.06728309052997	−1.32989906211664	c
10.99477575488040	3.14027647682439	−1.98512593710177	n

Table S9 Cartesian coordinates in a.u. of the optimized ground state minimum S_0-Min-2 at MP2/cc-pVDZ level of theory.

−5.70435756069744	−0.21848977035534	−1.43313051008141	c
−4.13831530125288	0.16614077328737	0.73485891037057	c
−4.42130670024349	2.23261887730351	2.38521582049891	c
−6.36383776761711	3.93760493577576	1.83657858657607	c
−7.96825629117554	3.59078352002191	−0.29064254528460	c
−7.66470367531930	1.53808363754573	−1.92319167942321	c
−3.17316312941390	2.46805314712267	4.01656494805091	h
−6.65397908954112	5.57457958492770	3.06881914112265	h
−9.47154722490566	4.96636776197765	−0.65107314321137	h
−8.90968784424083	1.29310080719668	−3.55890397119001	h
−2.42590042040789	−1.81013330785490	0.80308571676925	n
−2.78722534151885	−3.37083792322609	−1.28186099249664	c
−4.81686117471020	−2.47328562359076	−2.67295822056570	c
−1.56805939600099	−5.00908671657844	−1.56684297259434	h
−5.58629966539075	−3.34687126091120	−4.37328512008158	h
−0.40222031575528	−1.87781028900363	2.46507826889850	n
−0.40075764305586	−3.51600962744460	3.48654662683550	h
1.98273963394740	−1.28995326009487	1.39599788640916	c
4.19823822607155	−2.15076746424782	2.59664889252834	c
2.16174701632110	0.28067720230143	−0.74796971246577	c
6.57627772973332	−1.46918223911041	1.66296738315523	c
4.05866374685901	−3.36260343320707	4.27072837067020	h
4.54040602118103	0.96124112336751	−1.68645557028210	c
0.44331987965202	0.96449184567118	−1.67285087768870	h
8.29424417972730	−2.14867059693704	2.59134300906157	h
4.68361430154668	2.17518731971993	−3.35419797033055	h
6.76046559655404	0.09370745266778	−0.49056787360551	c
9.20773959150569	0.79255743062563	−1.46701587995657	c
11.22487546666102	1.36497522156357	−2.26968235085533	n

Table S10 Cartesian coordinates in a.u. of the optimized ground state minimum S_1-Min-a at ADC(2)/cc-pVDZ level of theory.

−5.88572168802383	−0.80998047129480	0.12199162521937	c
−3.25281607743825	−0.24758873623779	0.09610542487308	c
−2.28483843377981	2.15887883445376	0.64387230942204	c
−4.07519791236601	4.03463811340101	1.23377369184429	c
−6.69350770846937	3.52117490758682	1.27155004095986	c
−7.63004264498201	1.10190430255715	0.71826024713327	c
−0.25891747272360	2.53380500064719	0.60927698995545	h
−3.40191658784377	5.93945448149380	1.67311528119097	h
−8.01590620239937	5.04054465244028	1.74161404105500	h
−9.66041253367171	0.70799513071748	0.74823973895540	h
−2.03257170196323	−2.55285213079710	−0.56629532614427	n
−3.85291199868570	−4.47039289332547	−0.93664242039937	c
−6.20168493601737	−3.45756503934885	−0.52960978542428	c
−3.23781627295691	−6.36725870563804	−1.45685798501351	h
−7.98340551061112	−4.48313562563982	−0.67562072361083	h
0.42820702866724	−2.94269776358597	−0.82374386969420	n
0.83038061155809	−4.79280089421482	−1.31727770573223	h
2.30083717426606	−1.01211478746247	−0.44643094136099	c
3.78626962888028	−1.19725767630236	1.84974218529255	c
3.50625021792908	−0.03512872273550	−2.70583139693100	c
6.13568580172188	−0.06090143510437	1.97890388524259	c
2.98011766443468	−2.13636692993800	3.51496402537573	h
5.85750127531073	1.09358180845257	−2.54629800555981	c
2.48672172638027	−0.08879411898404	−4.51205475348203	h
7.19912022170427	−0.09252741872688	3.75682446795188	h
6.70784158402039	1.94572783183872	−4.23259822216387	h
7.23288350514974	1.16338060522219	−0.19459888542021	c
9.63910486820580	2.35407605991409	−0.03864366629776	c
11.66006459399519	3.36396235159354	0.09485072365494	n

Table S11 Cartesian coordinates in a.u. of the optimized ground state minimum S_1-Min-b at ADC(2)/cc-pVDZ level of theory.

−5.13750499700607	−0.39076121438008	−0.07535972352194	c
−2.44425409638942	−0.50817209859406	−0.06253961002198	c
−0.91234271809276	1.64747201719168	0.11971092368703	c
−2.18779111102376	3.97687231862528	0.29278902728583	c
−4.84815988940938	4.13733827508237	0.28380780799730	c
−6.35547184747903	1.95959706538669	0.09959165570120	c
1.14472331205379	1.57948503323309	0.13097217119917	h
−1.05484911804296	5.70009933238364	0.43771062852703	h
−5.75263343022312	5.99224846835292	0.42287591500317	h
−8.42030837646780	2.08289432429842	0.09184927385844	h
−1.84347967116189	−3.12209148245487	−0.26289513051262	n
−4.08836910507420	−4.56444808251190	−0.39406800136345	c
−6.10853333082187	−2.94852681400725	−0.28380138052613	c
−3.96786747146587	−6.61617022135653	−0.55336236839288	h
−8.09130778873359	−3.50925914827993	−0.34411818605871	h
0.44254535079133	−4.17435006725783	−0.32770217672249	n
0.34193342909899	−6.10316920042064	−0.47945034364724	h
2.80228327501586	−2.82534143358281	−0.20251630400526	c
3.55091928270471	−1.85968177379223	2.24817109232356	c
3.58856736101484	−1.48830738383345	−2.45919180721746	c
5.14602873832112	0.20205040548972	2.41016223711852	c
2.90952675204147	−2.82923886241735	3.96709016265490	h
5.18331062279199	0.57139678397953	−2.27046330028932	c
2.97604171248998	−2.17564038358560	−4.31891024331634	h
5.79846563587901	0.86147804121606	4.26340675876080	h
5.86428387998870	1.51298562484843	−3.98644545018408	h
5.96302533550346	1.53750196050163	0.16714117656088	c
7.53203706160437	3.71043426080103	0.34998030274426	c
8.83385300876192	5.55726757917290	0.50312447832306	n

Table S12 Cartesian coordinates in a.u. of the optimized ground state minimum S_1-Min-c at ADC(2)/cc-pVDZ level of theory.

−5.88161206166736	−0.71233274018942	−0.91854574194391	c
−4.07141691794527	0.21859076520488	0.83271538669456	c
−4.70427721819156	1.30823567988959	3.15312612757297	c
−7.29830114573001	1.45910946626155	3.72048919918057	c
−9.13780362616232	0.54929511812120	2.01556794208850	c
−8.46139435820668	−0.54101751576748	−0.31013070122039	c
−3.29223956070829	2.01882539297076	4.48750640691685	h
−7.88951029966115	2.29727554694018	5.51513162699325	h
−11.13735447145122	0.69873780978683	2.52130363618434	h
−9.90596773387728	−1.23926287504640	−1.61523229477150	h
−1.67536774954245	−0.20500306771126	−0.28086189654439	n
−1.95918298706191	−1.36966939645061	−2.66590696331397	c
−4.50123592401262	−1.69280291503655	−3.08554143504335	c
−0.25108581523309	−1.80251939317203	−3.73060193312209	h
−5.32027185490416	−2.54607287412182	−4.77302689737334	h
0.53160668417655	0.38790893285888	0.73135745020680	n
0.37655197335215	1.22823817028351	2.48519716878448	h
2.90266544079818	−0.11733202727014	−0.55198740508551	c
4.41332390051030	−2.11049652369321	0.58577751951894	c
4.20794116085564	2.12321334623509	−1.46054221559265	c
7.01622218535991	−2.06784729388315	0.37429603329087	c
3.46302652789106	−3.71315111228928	1.49906778110073	h
6.81228646515228	2.13586065685455	−1.65761019504649	c
3.10108136511725	3.75379965316462	−2.10996853892660	h
8.13647515733810	−3.64849932630307	1.10912790202783	h
7.77612371735080	3.77561413283504	−2.47955189663174	h
8.30397786313350	0.02962396036472	−0.79025264756288	c
10.98567344765430	0.05468505536638	−1.00624740841494	c
13.24067522133810	0.07343156732193	−1.19088402281856	n

Table S13 Cartesian coordinates in a.u. of the optimized ground state minimum S_1-Min-d at ADC(2)/cc-pVDZ level of theory.

−4.65659792151371	−1.76230887240466	−0.12271362592944	c
−3.79559317401041	0.64129127133825	0.70548849639707	c
−5.38500813292846	2.52418229923083	1.65007005944446	c
−7.97793970711383	1.93734122366398	1.76121468796811	c
−8.88717095619229	−0.43578769677278	0.95240892927067	c
−7.25218212904736	−2.30535143238557	0.00605573180247	c
−4.69871099130196	4.37157261291678	2.28119651565177	h
−9.30126688189109	3.35000154118474	2.48651551472718	h
−10.91464523509553	−0.82650346238010	1.06562591322464	h
−7.98304737303015	−4.13775460211339	−0.61526438043483	h
−1.13891969798772	0.64046477910632	0.35768029359745	n
−0.34005559337258	−1.69628460687557	−0.66312434225529	c
−2.45338679898141	−3.17675687352637	−0.96532046343864	c
1.66134495736258	−2.00167217383704	−1.04464913020882	h
−2.44470412955287	−5.09560885981413	−1.71663969969828	h
0.41368335475027	2.53416312811975	0.88943968425664	n
−0.47273591927039	4.08102051753196	1.63826524772599	h
3.13017334612350	2.34814513424491	0.47701657382086	c
4.41610781113774	0.61993914508915	2.18683877040298	c
3.86865692554109	2.31908717921128	−2.17151639277060	c
6.48065167635795	−0.75709435636011	1.37380600550702	c
3.79519892474796	0.49971875957909	4.16400335016765	h
5.93667515962841	0.93080308049622	−2.95609880658977	c
2.82804428286885	3.49764772098458	−3.52689590397572	h
7.51733761285431	−1.94956833567417	2.71530044803575	h
6.55706622732443	1.03058169909141	−4.93127241230665	h
7.30915321482763	−0.66938046772104	−1.22400789173952	c
9.40335064579879	−2.13395273471267	−2.05815392265446	c
11.15695019695347	−3.37902605892213	−2.76458182140641	n

Table S14 Cartesian coordinates in a.u. of the optimized ground state minimum S_0-Min-1 at COSMO-ADC(2)/cc-pVTZ level of theory in 1-chlorbutan.

−5.08458663231029	−0.45874380886126	−1.22719524970870	c
−3.08053939622236	−0.28038984363027	0.55127630375726	c
−2.52965533570726	1.92040748754240	1.89943142391640	c
−4.07757533663373	3.99363001507602	1.45815381991016	c
−6.10321087867924	3.86506621770941	−0.27265027783584	c
−6.62395898432681	1.67273465715236	−1.61443326820754	c
−0.97027446900089	2.00968361020525	3.22282689261553	h
−3.72148738902933	5.74297150094685	2.45753292347863	h
−7.26862604585705	5.52226907696378	−0.55883053223401	h
−8.18077369848348	1.60737806727375	−2.94255279540959	h
−1.90477896821478	−2.59971384874291	0.59651378754030	n
−3.03135983498515	−4.19900012386272	−1.12156007060003	c
−5.01311552020927	−2.95494584749584	−2.25967222816940	c
−2.31186062512180	−6.09163775662376	−1.35193252334218	h
−6.26698908471703	−3.75039933236831	−3.65519755306736	h
0.31743798539398	−3.14725874913052	1.85230560573391	n
0.06763291012064	−3.17319214126801	3.75294149202690	h
2.43754771893995	−1.76019846542485	1.05290076332922	c
4.49195533740219	−1.49331313538931	2.69371875986542	c
2.54973147492974	−0.75070252695765	−1.38597670853896	c
6.65242109946532	−0.23419673819386	1.90749188854847	c
4.39287500356601	−2.27102496241688	4.58517364975264	h
4.70907148568200	0.51182332465488	−2.18110066657165	c
0.95880971054992	−0.95308887260662	−2.65666538925361	h
8.24000157612195	−0.02104264430500	3.17805801483311	h
4.79992730484435	1.29659092858774	−4.06700308853096	h
6.76437059853534	0.77315520504726	−0.53782341858169	c
8.98199940650243	2.07692583847961	−1.35345837651796	c
10.80501058744460	3.14621305661098	−2.02227317873851	n

Table S15 Cartesian coordinates in a.u. of the optimized ground state minimum S_0-Min-1 at COSMO-CC2/cc-pVTZ level of theory in 1-chlorbutan.

−5.07328330447262	−0.45420348347033	−1.23719576418424	c
−3.09353696184245	−0.27568277315190	0.57146530805788	c
−2.55619966309232	1.92207976947871	1.92854597451426	c
−4.10236886288544	4.00062781545849	1.46837631566078	c
−6.10760207192885	3.87301516837142	−0.28652975667474	c
−6.61043885695883	1.67589565310460	−1.64016162139919	c
−1.01010536000361	2.00922695386610	3.26973843823571	h
−3.75666556042137	5.75009358702712	2.47333554705657	h
−7.27190606520899	5.52982716713845	−0.58605790179581	h
−8.15153359231795	1.61098469549807	−2.98839327714828	h
−1.91549504681396	−2.60494804684228	0.63436473475246	n
−3.01502082371385	−4.20082960949243	−1.12083558018056	c
−4.98256671031453	−2.95229138069780	−2.28043783316441	c
−2.28608781495305	−6.09148859745977	−1.34788433365469	h
−6.21946010884194	−3.74208119424584	−3.69609400951432	h
0.31966336145442	−3.13506918602721	1.88169499837080	n
0.08365678371581	−3.19444518122759	3.78560302828884	h
2.43332335684722	−1.75614714476310	1.07128485002346	c
4.50773011183466	−1.50562844758990	2.70134822035904	c
2.52445639267549	−0.73419332858403	−1.37099505976096	c
6.66638052507950	−0.25302730404228	1.89533461751232	c
4.42032429671016	−2.29009161727759	4.59174886844962	h
4.68626760381009	0.51944634154182	−2.17778723068090	c
0.91811511450711	−0.92236462170445	−2.62645671857311	h
8.26773679850091	−0.05254488717036	3.15284754160672	h
4.76404843851922	1.31203950623631	−4.06252570819447	h
6.76644133057261	0.76724368679279	−0.55252087571749	c
8.97948803878388	2.06177988928221	−1.38244498159249	c
10.81463865075864	3.13277675892328	−2.06936779065277	n