

Supplementary information

**Chiral conversion and periodical decay in bridged-
azobenzene photoisomerization: an ab initio on-the-fly
nonadiabatic dynamics simulation**

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Figure S1. Time evolution of potential energies of the S_1 and S_0 states and important angles involve in the photoisomerization for (a) trans to trans (nonreactive), (b) cis to cis (counterclockwise nonreactive), (c) cis to cis (clockwise nonreactive)

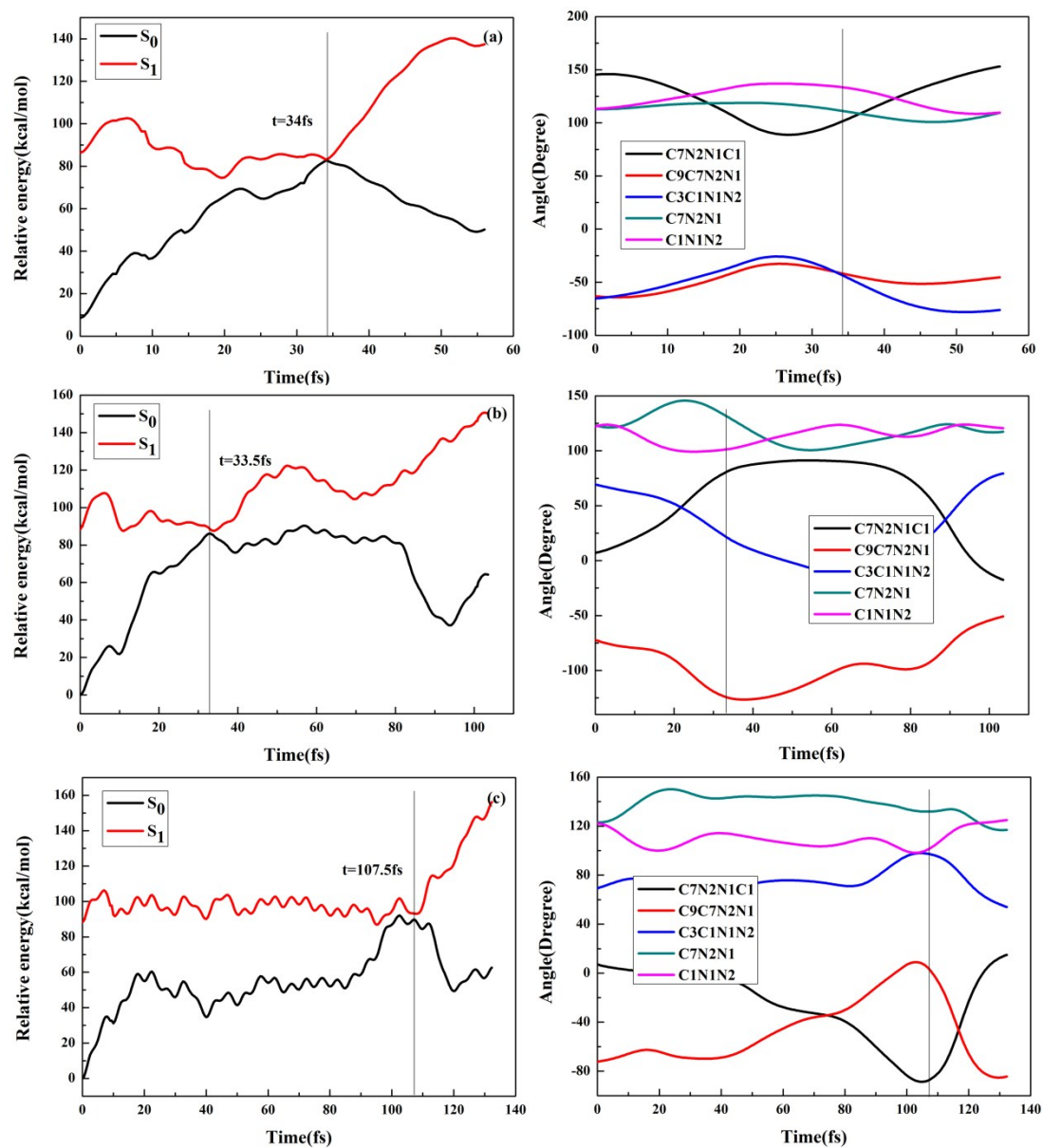


Table S1. Relative energies (kcal/mol) for the critical structures in the S₀ and S₁ states.

	(6e,5o)/6-31G ^a				(10e,8o)/6-31G ^a			
	cis	trans	CI-cis	CI-trans	cis	trans	CI-cis	CI-trans
CASSCF (S ₀ /S ₁)	0/88.3	8.6/86.3	48.9/49.0	46.9/47.1	0/71.9	16.4/74.6	56.3/56.8	42.4/42.4
CASPT2 (S ₀ /S ₁)	0/81.9	9.5/74.6	48.3/50.6	45.2/46.9	0/69.1	10.7/65.7	47.5/52.1	39.0/43.2
ICMRCI (S ₀ /S ₁)	0/87.4	8.8/83.5	49.9/50.8	48.8/49.6	0/72.8	14.6/73.5	53.2/56.9	45.5/50.6
	CASSCF (6e,5o)/6-31G ^c		CASSCF (10e,8o)/6-31G ^{*c}		CASSCF (14e,12o)/6-31G ^{*c}		Expt ^d	
	cis	trans	cis	trans	cis	trans	cis	trans
S ₀ Energy	0	8.8	0	7.1	0	7.1		
VEE ^b	88.2	77.7	80.6	69.2	80.3	68.7	70.8	58.4
	CASPT2(14e,12o)/app-TZ ^e				DFTB/6-31G ^{*f}		B3LYP/6-31G ^{*f}	
	cis	trans	CI-trans	CI-cis	cis	trans	cis	trans
S ₀ Energy	0	10.5	41.4	56.3	0	10.2	0	6.7
VEE ^b			2.3	9.5	62.7	50.7	67.3	55.5

^a This work^b Vertical Excitation Energies^c Ref.27.^d Ref.19.^e Ref.22.^f Ref.23.

Table S2. Cartesian coordinates for all optimized geometries**cis-b-Ab (S₀) CASSCF(6,5)**

N	1.70768642	1.06604894	0.31455858
N	1.68094222	-0.13012873	0.72264833
C	2.90555618	1.66980959	-0.21554228
C	3.44932023	2.75300898	0.45323068
C	3.40359467	1.24419744	-1.44178315
C	4.54545962	3.40763244	-0.08488377
C	4.49137332	1.92622472	-1.97658546
C	5.06605060	2.99340858	-1.30290673
C	2.86519140	-0.95657843	0.83904662
C	3.17293083	-1.27680650	2.17913109
C	3.58232086	-1.49976623	-0.20257170
C	4.22583456	-2.11011330	2.47730054
C	4.65380828	-2.36368480	0.13173104
C	4.97764431	-2.66410096	1.42505345
C	2.76128820	0.07174073	-2.14359044
C	3.30748423	-1.29885117	-1.68403170
H	4.24072921	-1.47828725	-2.20519585
H	2.61837707	-2.06911905	-2.02190177
H	3.01120695	3.07848097	1.37649948
H	4.97935289	4.24008851	0.43375332
H	4.88727420	1.62059325	-2.92699752
H	5.90656442	3.50505437	-1.73032500
H	2.55713306	-0.86343779	2.95365662
H	4.46123559	-2.34506612	3.49683538
H	5.22797172	-2.79113012	-0.66853569
H	5.79808633	-3.32199267	1.63708762
H	2.92958622	0.15313421	-3.21109940
H	1.68851863	0.10674450	-2.00296024

trans-b-Ab (S₀) CASSCF(6,5)

N	4.04581619	0.99454513	0.85536375
N	3.00596469	0.27527027	0.98788228
C	3.89362101	2.03353898	-0.10969256
C	4.04924062	3.36143806	0.15571479
C	3.72021019	1.53349541	-1.42803058
C	3.99487010	4.28453225	-0.90292331
C	3.69083640	2.46376377	-2.45226468
C	3.81958180	3.84172499	-2.18728304
C	3.31102697	-1.09171719	1.26129637
C	2.84013165	-1.77041731	2.36606537
C	4.00512369	-1.72873349	0.22568430
C	3.09819270	-3.12873101	2.48726901
C	4.23312577	-3.09287368	0.36468342
C	3.79434247	-3.78676719	1.48593119
C	3.54501750	0.03673009	-1.71736826
C	4.51078147	-0.98040281	-1.01497880
H	5.44186944	-0.48126655	-0.77358037
H	4.75836662	-1.73782632	-1.74959093
H	4.21023899	3.69353784	1.16263490
H	4.10008807	5.33196763	-0.69724385
H	3.56580739	2.13380482	-3.46647546
H	3.78727089	4.54010473	-3.00114748

H	2.28492000	-1.24403684	3.11754454
H	2.75121657	-3.66547458	3.34855119
H	4.75780130	-3.62046350	-0.40950373
H	3.98764235	-4.83888763	1.56859511
H	3.68013152	-0.08668877	-2.78565446
H	2.51966835	-0.24539353	-1.50951202

cis-b-Ab (S₀) CASSCF(10,8)

N	1.69130169	1.04544942	0.29764037
N	1.65602058	-0.15141604	0.70336552
C	2.89876315	1.64444646	-0.20929044
C	3.44108133	2.73232161	0.47503891
C	3.41456212	1.22435175	-1.43714105
C	4.55114412	3.38471649	-0.05124189
C	4.51997700	1.90893502	-1.95245589
C	5.08715602	2.96506379	-1.27086192
C	2.84744361	-0.96481818	0.83930801
C	3.17119284	-1.25912999	2.15903660
C	3.57537555	-1.50756183	-0.21808825
C	4.25332331	-2.06414444	2.45770547
C	4.65948072	-2.32491429	0.11145052
C	5.00396898	-2.60102761	1.42212593
C	2.76734963	0.06814424	-2.16123276
C	3.25455939	-1.32427324	-1.69220441
H	4.15404908	-1.57103752	-2.24340204
H	2.50846769	-2.05882298	-1.98474965
H	2.99303439	3.05651193	1.39402117
H	4.98438891	4.21441531	0.47235578
H	4.92742421	1.60437610	-2.89849068
H	5.93632888	3.47420578	-1.68434513
H	2.55655084	-0.85494071	2.93951107
H	4.50110105	-2.27567935	3.47939584
H	5.24255449	-2.74980802	-0.68353108
H	5.84579801	-3.23186054	1.63232951
H	2.96787854	0.14923947	-3.22313378
H	1.69224608	0.13436143	-2.05149369

trans-b-Ab (S₀) CASSCF(10,8)

N	4.04066505	0.99895231	0.86223704
N	3.00261892	0.27489227	0.98195028
C	3.89135127	2.03229363	-0.10918299
C	4.05090714	3.36048460	0.15482376
C	3.71663093	1.53245949	-1.42777223
C	3.99719314	4.28352380	-0.90344767
C	3.68815230	2.46300288	-2.45198757
C	3.81924454	3.84063969	-2.18757770
C	3.30370132	-1.08912422	1.26926945
C	2.84299232	-1.76123030	2.36255396
C	4.00466783	-1.73581733	0.21595418
C	3.10428398	-3.13655626	2.48514701
C	4.22962488	-3.09447001	0.35450962
C	3.78678798	-3.79294742	1.49512603
C	3.54451774	0.03595326	-1.71931449
C	4.51463592	-0.97536274	-1.01522121

H	5.43690969	-0.46692333	-0.76023161
H	4.77912306	-1.72564691	-1.75127720
H	4.21366469	3.69212601	1.16163090
H	4.10455868	5.33080445	-0.69814276
H	3.56231575	2.13311614	-3.46611601
H	3.78709816	4.53887495	-3.00157774
H	2.28902980	-1.24056363	3.11897224
H	2.75903672	-3.66558578	3.35198385
H	4.75173371	-3.62794262	-0.41745270
H	3.98127029	-4.84488374	1.57739787
H	3.68037623	-0.08596744	-2.78764789
H	2.51981262	-0.24932815	-1.51263970

S₀/S₁ CI-trans-1 CASSCF(6,5)

N	3.6877978198	1.3719069445	1.1635805813
N	2.9499421974	0.2699663863	1.3076016791
C	3.7721185092	2.0597423793	-0.0625354290
C	4.0756107644	3.4127420159	0.0766235053
C	3.5938255775	1.5048123853	-1.3635063927
C	4.1628027900	4.2495454644	-1.0418832808
C	3.6869025420	2.3510872926	-2.4399530034
C	3.9569809677	3.7233840403	-2.2906490323
C	3.3114085827	-1.0958519024	1.2708386018
C	2.8259421198	-1.8798163996	2.3119083974
C	4.0554475857	-1.6688933782	0.2357614732
C	3.0966559154	-3.2368765517	2.3532040792
C	4.3161662487	-3.0336688668	0.2962966047
C	3.8492351736	-3.8155441938	1.3426975260
C	3.3914207547	0.0241306150	-1.5728088778
C	4.5196974086	-0.8421173822	-0.9380293987
H	5.3386807688	-0.1985468435	-0.6318050323
H	4.9274750379	-1.5067505165	-1.6892662956
H	4.2230252434	3.7939387756	1.0670131308
H	4.3846534483	5.2908937069	-0.9137065736
H	3.5650616050	1.9512997425	-3.4290689511
H	4.0153754162	4.3470908405	-3.1620261289
H	2.2455406902	-1.4058758309	3.0775565294
H	2.7228965864	-3.8333251646	3.1624467490
H	4.8811413394	-3.4904070619	-0.4944011674
H	4.0609681163	-4.8674990132	1.3602242924
H	3.3547150030	-0.1659265841	-2.6380833919
H	2.4313411602	-0.2846694807	-1.1760600439

S₀/S₁ CI-trans-2 CASSCF(6,5)

N	4.0800094498	1.2441915133	1.0463702683
N	3.2785474614	0.3453777282	1.6107832516
C	3.9205901271	2.0320004681	-0.1184569639
C	4.0528517884	3.4057219257	0.0475999100
C	3.7094750216	1.4827247171	-1.3850169547
C	3.9445168309	4.2555035261	-1.0389440905
C	3.6056105759	2.3553449606	-2.4638472323
C	3.7144721123	3.7273926143	-2.3001756213
C	3.4386211465	-1.0306305272	1.3890785433
C	2.8348786397	-1.8262864450	2.3630246430

C	4.1248964412	-1.6451112871	0.2997213709
C	2.9165621826	-3.2191670645	2.3078942549
C	4.1912093151	-3.0159046969	0.2780313952
C	3.6012296716	-3.8100273941	1.2765315976
C	3.6143811930	-0.0095713982	-1.5982801881
C	4.6929005096	-0.8418445835	-0.8459216813
H	5.4845302397	-0.1893382001	-0.4984961199
H	5.1510720896	-1.5316754364	-1.5434907407
H	4.2343440869	3.7848994784	1.0328297690
H	4.0410812540	5.3145332676	-0.9016932734
H	3.4470766215	1.9510187197	-3.4458981066
H	3.6322350619	4.3748682032	-3.1514330780
H	2.3166827716	-1.3315078310	3.1595570015
H	2.4512554427	-3.8128397328	3.0699637295
H	4.6971893640	-3.4998730469	-0.5360747736
H	3.6819090066	-4.8780081360	1.2165684667
H	3.6949367608	-0.2041498629	-2.6605705695
H	2.6282821608	-0.3579747791	-1.3061308038

S₀/S₁ CI-trans-3 CASSCF(6,5)

N	3.0275114791	1.3307200412	1.1806120379
N	3.7771765483	0.3116948549	1.6413673736
C	3.4475278352	2.0827625069	0.0260849189
C	3.5186040190	3.4509725134	0.2589957104
C	3.7032291081	1.5637469613	-1.2450525248
C	3.8884072157	4.3231712207	-0.7496159937
C	4.0555967083	2.4612650770	-2.2510896489
C	4.1591850302	3.8225578148	-2.0130965270
C	3.6528939915	-1.0834215741	1.3778178662
C	3.1534137468	-1.8576066077	2.3952832493
C	4.1013331588	-1.6741062600	0.1739605074
C	3.0386313379	-3.2458391779	2.2377097154
C	3.9931564827	-3.0487275488	0.0419063782
C	3.4607633227	-3.8380697545	1.0757405492
C	3.5703087758	0.0959506230	-1.5808561432
C	4.6515646404	-0.8188664927	-0.9382649214
H	5.4704537615	-0.2121602727	-0.5684888338
H	5.0674640237	-1.4664462039	-1.7003214331
H	3.2780839329	3.8099412724	1.2396365284
H	3.9538050169	5.3754650245	-0.5538106642
H	4.2460868318	2.0836808183	-3.2378815414
H	4.4361535022	4.4844326308	-2.8108365874
H	2.8593893293	-1.3847747764	3.3108072968
H	2.6285485671	-3.8353981388	3.0344626606
H	4.3231013354	-3.5191113545	-0.8652687316
H	3.3936674281	-4.9015898699	0.9504527225
H	3.6238693978	-0.0035810553	-2.6577042287
H	2.5849340229	-0.2572631804	-1.2959582954

S₀/S₁ CI-trans-4 CASSCF(6,5)

N	3.0611341420	1.2270836942	1.0805697490
N	3.7751736544	0.3113092675	1.7604595302
C	3.4500729881	2.0569600244	-0.0080621992
C	3.5249173728	3.4036594142	0.2543577656
C	3.6849859225	1.5629946509	-1.3143067731

C	3.8725014651	4.3095564280	-0.7567202500
C	4.0213469581	2.4767965592	-2.3003985017
C	4.1220075364	3.8508963126	-2.0236785425
C	3.6455243450	-1.0825361878	1.4189044634
C	3.1572621512	-1.8878608768	2.4391696872
C	4.0549727360	-1.6338531576	0.2060257341
C	3.0256682982	-3.2533487594	2.2529623873
C	3.9331546688	-3.0119962828	0.0450524907
C	3.4161818957	-3.8171388169	1.0480518069
C	3.5694956493	0.0922999459	-1.6303174749
C	4.6275769221	-0.7876229943	-0.9059842770
H	5.4200662914	-0.1556409375	-0.5198425045
H	5.0926220765	-1.4470090947	-1.6281811699
H	3.3118380177	3.7475109086	1.2463644228
H	3.9365072445	5.3560209958	-0.5302253114
H	4.2071716084	2.1260867525	-3.2980213662
H	4.3891259315	4.5322347830	-2.8082495132
H	2.8891195528	-1.4283347080	3.3695581713
H	2.6363160249	-3.8679298413	3.0408893202
H	4.2527974985	-3.4572626831	-0.8782523206
H	3.3312833768	-4.8754785023	0.8932699217
H	3.6736651195	-0.0353635518	-2.7007263292
H	2.5758324562	-0.2596911120	-1.3755901131

S₀/S₁ CI-cis-1 CASSCF(6,5)

N	-1.1471995296	1.1669741795	-0.4983953366
N	-1.4779483753	0.5072082284	0.6034698691
C	-0.5876792262	0.4149441624	-1.5710816886
C	-0.3264641605	1.1847225774	-2.7009941256
C	-0.2827724540	-0.9522252752	-1.5479929241
C	0.2518631736	0.6259628104	-3.8242907477
C	0.2937123616	-1.4936269655	-2.6967972134
C	0.5638552608	-0.7252753842	-3.8180774151
C	-0.6900861669	0.3342277477	1.7698395950
C	-0.8816650218	1.2443474827	2.8326482817
C	0.2049132269	-0.7049168438	1.8737663121
C	-0.1510607625	1.1174444998	3.9918629097
C	0.9437817667	-0.8141876454	3.0753146878
C	0.7808951793	0.0676128903	4.1072671684
C	-0.5373616698	-1.8799282183	-0.3721894557
C	0.4584059588	-1.7530882427	0.8032341533
H	1.4558786037	-1.6051883532	0.3980660778
H	0.4827852181	-2.7139669965	1.3087673525
H	-0.5886957734	2.2231585679	-2.6670529768
H	0.4501986528	1.2291058088	-4.6883329530
H	0.5309989712	-2.5404941480	-2.7109598162
H	1.0084463369	-1.1816722736	-4.6813948151
H	-1.6027992464	2.0271757932	2.7087013831
H	-0.2910980427	1.8084565969	4.7999557690
H	1.6486680816	-1.6194886720	3.1700727326
H	1.3555829780	-0.0427694644	5.0065781245
H	-0.4432063159	-2.8924328672	-0.7481589253
H	-1.5522977490	-1.7801424687	-0.0139614306

S₀/S₁ CI-cis-2 CASSCF(6,5)

N	0.0000418259	-0.0012052824	-0.0005049798
N	0.0001117017	-0.0007322498	1.3257213120
C	1.2641971220	-0.0003175409	-0.6570939334
C	1.1604204998	0.0568731531	-2.0439771946
C	2.5166718135	-0.0746757574	-0.0337543100
C	2.2868372102	0.0290231004	-2.8433190679
C	3.6382863120	-0.0946319399	-0.8625000608
C	3.5349813660	-0.0479558952	-2.2437046514
C	-0.0922588720	-1.1252047317	2.1847884020
C	-1.3719728059	-1.4832499813	2.6631953502
C	1.0311632991	-1.8214282667	2.5648460442
C	-1.5184718814	-2.5598570489	3.5079550912
C	0.8546941346	-2.9238739471	3.4337183189
C	-0.3789056050	-3.2924996684	3.8936053548
C	2.7380958095	-0.1302277903	1.4682161441
C	2.4513119208	-1.4957233846	2.1334303373
H	2.8062770566	-2.2836353353	1.4744681241
H	3.0681807791	-1.5542369199	3.0253364976
H	0.1780703558	0.1221489054	-2.4671098433
H	2.1947065358	0.0719159857	-3.9107236784
H	4.6117899118	-0.1439711735	-0.4126293800
H	4.4237928883	-0.0651973424	-2.8446355974
H	-2.2140275870	-0.8990520799	2.3503145058
H	-2.4888320912	-2.8369966044	3.8710387189
H	1.7231239459	-3.4788757138	3.7372980422
H	-0.4797248077	-4.1331484107	4.5526638871
H	3.7883123257	0.0800842442	1.6360636139
H	2.1860559961	0.6523126556	1.9694193227

S₀/S₁ CI-trans-1 CASSCF(10,8)

N	3.5645928786	1.3756871467	1.1451398506
N	2.9249769896	0.2518195185	1.2544047940
C	3.6992965144	2.0728038049	-0.0637157007
C	4.0096618889	3.4382201061	0.0892603123
C	3.5760364514	1.5135789872	-1.3540460904
C	4.1654220528	4.2532084093	-1.0006720346
C	3.7395013607	2.3703819225	-2.4508562560
C	4.0229924192	3.7250242914	-2.2877035921
C	3.2900804342	-1.1074581533	1.2699061944
C	2.8422610227	-1.8773418080	2.3368331059
C	4.0181431430	-1.6834676385	0.2253363125
C	3.1364106364	-3.2287613810	2.3930376468
C	4.3064096084	-3.0418486708	0.3054873708
C	3.8772777939	-3.8118466629	1.3761546268
C	3.3541063719	0.0342210730	-1.5839734279
C	4.4639058690	-0.8667920094	-0.9653951991
H	5.3117878353	-0.2479219779	-0.6877300612
H	4.8290311969	-1.5491291937	-1.7230252575
H	4.1059836975	3.8155351349	1.0876376138
H	4.3927384731	5.2930085959	-0.8673981158
H	3.6539571648	1.9652821993	-3.4416737693
H	4.1399900990	4.3556550316	-3.1475792640
H	2.2741253895	-1.3998944266	3.1093752414

H	2.7927594495	-3.8172588172	3.2211381949
H	4.8650918525	-3.5027083771	-0.4872668412
H	4.1120614860	-4.8581392746	1.4098150290
H	3.3277201052	-0.1352472097	-2.6533748652
H	2.3850251426	-0.2669439205	-1.2055918143

S₀/S₁ CI-trans-2 CASSCF(10,8)

N	3.6416083774	1.2585649844	1.0290589954
N	2.8878600971	0.2654280745	1.3853491383
C	3.7436909505	2.0459874698	-0.1019327050
C	4.0738416453	3.3997508916	0.0707520537
C	3.5792926857	1.5176161600	-1.4014370583
C	4.1940898385	4.2298683075	-1.0221476298
C	3.6960454533	2.3804057661	-2.4775286425
C	3.9929990871	3.7274014455	-2.3036391127
C	3.2941277647	-1.0870644225	1.3149620347
C	2.8187624421	-1.9045455412	2.3489338466
C	4.0432662811	-1.6411334507	0.2592247256
C	3.1211049087	-3.2480423877	2.3781096367
C	4.3238044339	-3.0006908366	0.3112944358
C	3.8853067719	-3.8009061151	1.3563197108
C	3.3687076808	0.0355423795	-1.5921796017
C	4.4919499822	-0.8238603302	-0.9327270676
H	5.3150591682	-0.1772326144	-0.6489912781
H	4.8894154880	-1.5070230031	-1.6728148114
H	4.2109010670	3.7677635120	1.0676783482
H	4.4359587610	5.2653758702	-0.8809924620
H	3.5723138323	1.9917603522	-3.4710632394
H	4.0789397518	4.3714228997	-3.1570410988
H	2.2256368483	-1.4502893211	3.1173138230
H	2.7648628128	-3.8621816077	3.1819443058
H	4.8872206095	-3.4437579151	-0.4882563655
H	4.1242097356	-4.8467261556	1.3647603404
H	3.3389068464	-0.1740352428	-2.6540258049
H	2.4029460512	-0.2646277506	-1.1989543675

S₀/S₁ CI-trans-3 CASSCF(10,8)

N	3.2473154109	1.3393476071	1.2355832444
N	3.9200931771	0.2717563457	1.5660918321
C	3.5321232855	2.1004256486	0.0708791306
C	3.5049975406	3.4890787269	0.2722410662
C	3.7816708430	1.5715047694	-1.2114118909
C	3.7799188617	4.3628438154	-0.7707786350
C	4.0533340662	2.4815170287	-2.2396156282
C	4.0672914588	3.8451992466	-2.0349085329
C	3.6973254888	-1.1138213120	1.3641366265
C	3.1409822233	-1.8634640005	2.3898323153
C	4.1199083845	-1.7116689866	0.1781828884
C	2.9765328148	-3.2307775208	2.2325030255
C	3.9545772426	-3.0851712075	0.0421416374
C	3.3857399973	-3.8419277573	1.0570365054
C	3.6588410301	0.1000953782	-1.5552097713
C	4.7058834071	-0.8620650761	-0.9215033805
H	5.5451475364	-0.2910499673	-0.5411706055
H	5.0970350878	-1.5134499924	-1.6934819762

H	3.2783726141	3.8496119325	1.2554586140
H	3.7702154449	5.4222780179	-0.6045553385
H	4.2430909598	2.0984875736	-3.2247106618
H	4.2832011713	4.5060743159	-2.8521828677
H	2.8500497820	-1.3708688172	3.2958996181
H	2.5408374955	-3.8111597363	3.0221433747
H	4.2744503297	-3.5648258388	-0.8636236429
H	3.2680103388	-4.9009216475	0.9312571091
H	3.7238114907	0.0155528584	-2.6329167874
H	2.6641030664	-0.2432023136	-1.2907258288

S₀/S₁ CI-trans-4 CASSCF(10,8)

N	2.8225934403	1.1721405865	0.8768758414
N	3.3577388131	0.3172512069	1.7042256511
C	3.3678972346	2.0596636700	-0.0849928959
C	3.5452596330	3.3930821042	0.2528483172
C	3.6318523996	1.5985478885	-1.3734609163
C	4.0159423959	4.2871990078	-0.6960172479
C	4.0951668923	2.5116811548	-2.3136166060
C	4.2894477487	3.8451662726	-1.9815068147
C	3.4769032939	-1.0674281131	1.4120081335
C	3.1494660870	-1.9104802566	2.4851623852
C	3.9216454888	-1.6103208058	0.1898240382
C	3.2015492263	-3.2905541979	2.3448000054
C	3.9630670500	-3.0054144129	0.0841651499
C	3.6028359002	-3.8362021363	1.1242213488
C	3.4421879801	0.1384506950	-1.7002169509
C	4.4586771458	-0.7770891439	-0.9571625615
H	5.2800251955	-0.1665220215	-0.5967305701
H	4.8923518702	-1.4614452306	-1.6757863157
H	3.3088997862	3.7139008441	1.2475567094
H	4.1595215722	5.3174479145	-0.4349082053
H	4.3035111375	2.1764250768	-3.3121108609
H	4.6471151571	4.5332000261	-2.7230029844
H	2.8475581645	-1.4556579489	3.4071377566
H	2.9357988896	-3.9272676146	3.1658115701
H	4.3016678587	-3.4386327054	-0.8382232485
H	3.6470078911	-4.9007938066	0.9976856060
H	3.5623803684	0.0025666763	-2.7680520855
H	2.4302532840	-0.1665724996	-1.4594554447

S₀/S₁ CI-cis-1 CASSCF(10,8)

N	-1.1283508190	1.1745799576	-0.5019080730
N	-1.4656279366	0.5204199004	0.6010668630
C	-0.5834869478	0.4252970529	-1.5737261767
C	-0.3289186002	1.1833954460	-2.6996253015
C	-0.2772238273	-0.9581393025	-1.5495048624
C	0.2447863621	0.6176617945	-3.8348739760
C	0.2905219417	-1.4998390352	-2.7025678167
C	0.5537947106	-0.7245223959	-3.8330128875
C	-0.6839346576	0.3391145857	1.7696963074
C	-0.8793011685	1.2465683946	2.8346236509
C	0.2087894657	-0.7016973299	1.8761858578
C	-0.1577776476	1.1140319377	3.9990842534
C	0.9374741022	-0.8173931815	3.0833116771
C	0.7701278560	0.0609918700	4.1174946018

C	-0.5299523739	-1.8797639361	-0.3681522734
C	0.4671374960	-1.7477044180	0.8048231307
H	1.4631385764	-1.5933960949	0.3978611609
H	0.4993503611	-2.7081622978	1.3106252908
H	-0.5864978175	2.2232327768	-2.6707929326
H	0.4373352723	1.2241209769	-4.6979560074
H	0.5290282264	-2.5465217160	-2.7210148725
H	0.9919889270	-1.1819808959	-4.6992262692
H	-1.5965882050	2.0324537340	2.7075941848
H	-0.3011221414	1.8033037455	4.8082011872
H	1.6383613007	-1.6258749315	3.1806087738
H	1.3381601841	-0.0542934409	5.0204185697
H	-0.4368167716	-2.8941004446	-0.7401781863
H	-1.5447445922	-1.7798452254	-0.0091912814

S₀/S₁ CI-cis-2 CASSCF(10,8)

N	0.0077986387	-0.0073126396	-0.0136088992
N	-0.0037446729	-0.0308354592	1.3059610362
C	1.2478400672	0.0007767922	-0.6657059365
C	1.1522535838	0.0831654835	-2.0586042144
C	2.5239594172	-0.0939345857	-0.0412100283
C	2.2896656259	0.0566233593	-2.8583753949
C	3.6278378001	-0.1107922782	-0.8662734928
C	3.5257429115	-0.0417502525	-2.2626232025
C	-0.1014183222	-1.1323114627	2.1860901022
C	-1.3805931530	-1.4675759047	2.6833581963
C	1.0170661547	-1.8374951997	2.5661381139
C	-1.5318782749	-2.5298308731	3.5453416322
C	0.8357888909	-2.9260307795	3.4511609107
C	-0.3977805435	-3.2721852701	3.9286506836
C	2.7412949242	-0.1671555108	1.4601894810
C	2.4364864809	-1.5332050378	2.1179365764
H	2.7718065770	-2.3218788964	1.4496289469
H	3.0623221592	-1.6082203362	3.0023358200
H	0.1727984872	0.1656302075	-2.4851256485
H	2.1983008593	0.1168113879	-3.9252603088
H	4.6046842280	-0.1756755272	-0.4249113855
H	4.4177916787	-0.0605857212	-2.8583328139
H	-2.2182113785	-0.8777132312	2.3693099981
H	-2.5016761644	-2.7893452416	3.9227299827
H	1.6999690461	-3.4882358540	3.7535888907
H	-0.5026166258	-4.1026965508	4.5998756421
H	3.7944061343	0.0270945060	1.6304850570
H	2.1997952403	0.6195360260	1.9671748951

TS-S₀ CASSCF(6,5)

N	0.4650246593	-1.2183433487	-0.0176580588
N	-0.6728479239	-1.6152994950	0.3236749146
C	1.7298908717	-0.6807065251	-0.0460593574
C	2.8340492577	-1.4179653033	-0.4585194472
C	1.8566971425	0.6562932881	0.3506410926
C	4.0833570342	-0.8186964589	-0.4766945878
C	3.1250010938	1.2181473408	0.3721286474
C	4.2330909219	0.4916400216	-0.0452877248
C	-1.8005548523	-0.7321542769	0.0669891358
C	-3.0123747345	-1.3498560129	0.2379083367

C	-1.7233027183	0.6489996043	-0.2576686332
C	-4.2129143256	-0.6457682909	0.0810402590
C	-2.9269493806	1.3274617080	-0.3945063913
C	-4.1675705393	0.6868321858	-0.2322356274
C	0.6012866787	1.4225534290	0.6870948230
C	-0.4311422313	1.4153346938	-0.4855858065
H	0.0564615184	1.0445493656	-1.3785669004
H	-0.7051849614	2.4418363141	-0.6983809820
H	2.7022198895	-2.4407290205	-0.7488163197
H	4.9372294907	-1.3795223726	-0.8036634952
H	3.2445964032	2.2373103627	0.6883640707
H	5.2039787953	0.9479257993	-0.0392326899
H	-3.0133976543	-2.3897498019	0.4988269269
H	-5.1507092459	-1.1493741766	0.2115838222
H	-2.9110410525	2.3737655893	-0.6352092870
H	-5.0726710085	1.2506262209	-0.3528502850
H	0.8668612498	2.4463372134	0.9216030783
H	0.1383946221	1.0181289466	1.5819324865

TS-S₀ CASSCF(10,8)

N	0.4661200831	-1.2333566387	0.0214969663
N	-0.6743923503	-1.5986255096	0.3865895513
C	1.7285912553	-0.6995945868	-0.0239965769
C	2.8177579603	-1.4199439578	-0.4574475792
C	1.8590155151	0.6564880448	0.3783012030
C	4.0764213640	-0.8047880039	-0.5068466988
C	3.1191481627	1.2234383771	0.3667393134
C	4.2334047799	0.4918159886	-0.0853611866
C	-1.7980264892	-0.7247669861	0.0935923674
C	-3.0115645399	-1.3434619868	0.2495450089
C	-1.7178118226	0.6521585803	-0.2473750794
C	-4.2103922906	-0.6458264120	0.0560086297
C	-2.9201774259	1.3248410590	-0.4191762468
C	-4.1619774044	0.6822918295	-0.2755168054
C	0.5991669180	1.4118881725	0.7247047930
C	-0.4229362520	1.4196596763	-0.4554439530
H	0.0709628845	1.0559749696	-1.3484007038
H	-0.6937885610	2.4481359892	-0.6622590934
H	2.6932068386	-2.4441614839	-0.7457047678
H	4.9206317405	-1.3664956527	-0.8571114334
H	3.2437128395	2.2461203228	0.6699595507
H	5.2003156577	0.9559192365	-0.1061901591
H	-3.0156881897	-2.3790010994	0.5272794967
H	-5.1492972136	-1.1504152787	0.1738475964
H	-2.9021219645	2.3682237165	-0.6719081699
H	-5.0659040252	1.2414700819	-0.4232397667
H	0.8589627624	2.4324118170	0.9789812463
H	0.1341387473	0.9891767446	1.6097845070