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

Supplementary material

Dynamic Effects of the Bridged Structure on the Quantum Yield of the *Cis*→*Trans* Photoisomerization of Azobenzene

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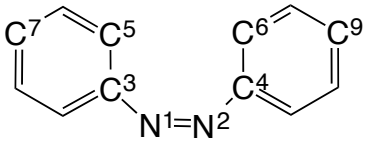
Table S1 Relative energies (kcal/mol) at the various levels of the *cis* and *trans* forms and the clockwise (CW) and counterclockwise (CCW) conical intersection (CI) in the *cis*→*trans* isomerization for azobenzene **1** and diindane diazocine **4**[a]

	Azobenzene **1**[b]			Diindane diazocine **4**		
	Level 1	Level 2	Level 3	Level 1	Level 2	Level 4
Cis	0.0	0.0	0.0	0.0	0.0	0.0
Trans-CCW	-8.9	-18.7	-18.6	6.3	2.1	3.5
Trans-CW	-8.9	-18.7	-18.6	4.1	5.9	
CI-CCW	42.1	41.5	38.9	35.7	36.6	
CI-CW	44.3	41.5	39.1	39.6	42.7	

[a]Level 1, CASSCF(6,5) with the basis set 6-31G for all the atoms; Level 2, CASSCF(10,8) with the basis set 6-31G(d) for the N atoms and 6-31G for the C and H atoms; Level 3, CASSCF(10,8) with the basis set cc-pVDZ for all the atoms; Level 4, PBE(D3(BJ)) with the basis set def2TZVP for all the atoms [Ref. 12]. [b]For azobenzene **1**, *Trans*-CCW and *Trans*-CW are the same structures.

Table S2 Optimized structural parameters (Å and degree) at the various levels of the S_1/S_0-CI in the *cis*→*trans* isomerization for azobenzene **1** and diindane diazocine **4** [a]



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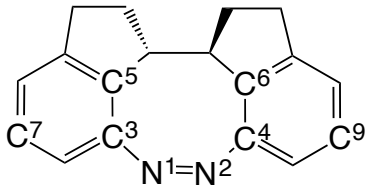

4

	Azobenzene **1**			Diindane diazocine **4**	
	Level 1	Level 2	Level 3	Level 1	Level 2
			Counterclockwise S_1/S_0-CI		
$d(N^1\text{-}N^2)$	1.311	1.285	1.287	1.347	1.300
$d(N^1\text{-}C^3)$	1.427	1.403	1.398	1.406	1.428
$d(N^2\text{-}C^4)$	1.373	1.376	1.375	1.440	1.388
$C^3\text{-}N^1\text{-}N^2$	117.4	117.0	117.4	117.4	116.9
$C^4\text{-}N^2\text{-}N^1$	131.5	131.2	130.7	124.6	130.6
$C^3\text{-}N^1\text{-}N^2\text{-}C^4$	90.8	91.6	91.6	94.8	95.4
$C^5\text{-}C^3\text{-}N^1\text{-}N^2$	-177.4	179.5	179.6	-70.2	-58.3
$C^6\text{-}C^4\text{-}N^2\text{-}N^1$	-0.2	-0.4	-0.4	-17.2	-25.2
			Clockwise S_1/S_0-CI		
$d(N^1\text{-}N^2)$	1.319	1.276	1.277	1.351	1.281
$d(N^1\text{-}C^3)$	1.394	1.380	1.379	1.421	1.385
$d(N^2\text{-}C^4)$	1.423	1.419	1.416	1.436	1.429
$C^3\text{-}N^1\text{-}N^2$	128.6	131.2	130.5	127.4	134.3
$C^4\text{-}N^2\text{-}N^1$	117.5	117.7	118.1	114.8	114.9
$C^3\text{-}N^1\text{-}N^2\text{-}C^4$	-91.0	-92.4	-92.4	-93.2	-95.1
$C^5\text{-}C^3\text{-}N^1\text{-}N^2$	-0.6	1.1	0.9	43.9	42.9
$C^6\text{-}C^4\text{-}N^2\text{-}N^1$	178.7	179.7	179.3	85.5	82.2

[a]Level 1, CASSCF(6,5) with the basis set 6-31G for all the atoms; Level 2, CASSCF(10,8) with the basis set 6-31G(d) for the N atoms and 6-31G for the C and H atoms; Level 3, CASSCF(10,8) with the basis set cc-pVDZ for all the atoms.

Table S3 Vertical excitation energies of $S_0 \rightarrow S_1$ at the various levels for azobenzene **1** and diindane diazocine **4**[a]

	Azobenzene **1**	Diindane diazocine **4**
Exp.	67.3[b]	66.3[c]
CASSCF		
(6e,5o)/6-31G	74.7	72.0
(6e,5o)/6-31G(d)	77.4	89.7
(6e,5o)/cc-pVDZ	77.2	89.7
(10e,8o)/6-31G	69.5	66.6
(10e,8o)/6-31G(d)	75.3	73.1
(10e,8o)/cc-pVDZ	75.1	72.6
MS-CASPT2		
(6e,5o)/6-31G	80.3	77.8
(6e,5o)/6-31G(d)	62.2	77.5
(6e,5o)/cc-pVDZ	61.4	75.5
(10e,8o)/6-31G	66.5	64.5
(10e,8o)/6-31G(d)	67.8	65.1
(10e,8o)/cc-pVDZ	67.0	63.6
XMS-CASPT2		
(6e,5o)/cc-pVDZ	56.8	66.1
(10e,8o)/cc-pVDZ	64.3	

[a]The structures optimized at the CASSCF(6,5)/6-31G level were used. [b]D. L. Beveridge and H. H. Jaffé, *J. Am. Chem. Soc*., 1966, **88**, 1948–1953. [c]Ref. 12

Table S4 Pattern of motion of all normal modes for azobenzene **1** with the *cis* form and the vibrational frequencies for each normal mode at the CASSCF(10,8)/cc-pVDZ level

Normal mode No.	Vibrational frequency (cm^{-1})	Pattern of motion
1	31.4	Rotation of Ph
2	59.5	Rotation of Ph
3	63.8	Butterfly motion of Ph
4	155.0	Twist of N_2
5	158.4	Butterfly motion of Ph
6	280.1	Butterfly motion of Ph
7	335.1	Wag of N_2
8	445.5	Twist of Ph
9	448.1	Twist of Ph
10	456.5	Twist of Ph
11	484.0	Bend of Ph
12	538.1	Bend of Ph
13	592.2	Bend of Ph
14	632.2	Bend of Ph
15	671.6	Deformation of Ph
16	675.8	Deformation of Ph
17	740.5	Bend of Ph
18	767.1	Bend of Ph
19	771.9	Bend of Ph
20	795.3	Bend of H
21	833.8	Bend of H
22	860.2	Bend of H
23	940.7	Bend of H
24	943.4	Bend of H
25	952.2	Bend of H, Rotation of N_2
26	1022.2	Bend of H
27	1039.0	Bend of H, Rotation of N_2
28	1083.2	Deformation of Ph
29	1083.9	Deformation of Ph

30	1088.4	Bend of H
31	1089.6	Bend of H
32	1106.3	Bend of H
33	1107.2	Bend of H
34	1115.9	Deformation of Ph
35	1118.6	Deformation of Ph
36	1166.0	Deformation of Ph
37	1168.0	Deformation of Ph
38	1206.5	Deformation of Ph
39	1211.9	Deformation of Ph
40	1224.0	Deformation of Ph
41	1271.7	Rocking of H
42	1274.0	Rocking of H
43	1296.3	Deformation of Ph
44	1322.4	Rocking of H
45	1327.0	Rocking of H
46	1435.8	Rocking of H
47	1440.9	Rocking of H
48	1585.8	Rocking of H, Stretch of N_2
49	1589.2	Rocking of H, Stretch of N_2
50	1600.5	Rocking of H, Stretch of N_2
51	1636.5	Rocking of H
52	1651.2	Rocking of H
53	1776.1	Stretch of Ph CC
54	1783.8	Stretch of Ph CC
55	1794.3	Stretch of Ph CC
56	1801.0	Stretch of Ph CC
57	3337.6	Stretch of Ph CH
58	3338.4	Stretch of Ph CH
59	3348.3	Stretch of Ph CH
60	3349.4	Stretch of Ph CH
61	3358.7	Stretch of Ph CH
62	3359.8	Stretch of Ph CH

63	3368.4	Stretch of Ph CH
64	3369.4	Stretch of Ph CH
65	3375.8	Stretch of Ph CH
66	3377.0	Stretch of Ph CH

Table S5 Pattern of motion of all normal modes for diindane diazocine **4** with the *cis* form and the vibrational frequencies for each normal mode at the CASSCF(6,5)/6-31G level

Normal mode No.	Vibrational frequency (cm^{-1})	Pattern of motion
1	54.3	Butterfly motion of 6-membered ring
2	81.5	Rotation of 6-membered ring
3	140.2	Twist of 5-membered ring
4	166.7	Twist of 5-membered ring
5	190.1	Twist of N_2
6	212.8	Butterfly motion of 6-membered ring
7	254.5	Bend of 5-membered ring
8	256.4	Bend of 5-membered ring
9	280.7	Deformation of 8-membered ring
10	310.5	Bend of 5-membered ring
11	355.7	Butterfly motion of 6-membered ring
12	426.1	Bend of 8-membered ring
13	436.0	Bend of 6-membered ring
14	451.3	Bend of 6-membered ring
15	502.7	Deformation of 6-membered ring
16	544.5	Bend of 6-membered ring
17	551.3	Bend of 6-membered ring
18	567.3	Bend of 6-membered ring
19	599.9	Bend of 5 and 6-membered rings
20	612.2	Bend of 6-membered ring
21	616.3	Bend of 6-membered ring
22	652.7	Bend of 6-membered ring
23	663.8	Bend of 6-membered ring, Deformation of 5-membered ring, Twist of N_2
24	672.1	Deformation of 5 and 6-membered rings
25	693.3	Deformation of 5 and 6-membered rings
26	731.2	Deformation of 5 and 6-membered rings
27	775.5	Deformation of 5 and 6-membered rings
28	808.7	Deformation of 5 and 6-membered rings

29	853.3	Deformation of 5 and 6-membered rings, Rocking of 6-membered ring H
30	865.2	Deformation of 5 and 6-membered rings, Rocking of 6-membered ring H
31	898.8	Deformation of 5 and 6-membered rings, Rocking of 6-membered ring H
32	908.3	Deformation of 5 and 6-membered rings, Rocking of 6-membered ring H
33	924.1	Bend of 6-membered ring H
34	933.5	Deformation of 5 and 6-membered rings
35	951.6	Deformation of 5 and 6-membered rings
36	985.3	Deformation of 5 and 6-membered rings
37	986.9	Stretch of CC
38	1012.8	Stretch of CC
39	1047.9	Stretch of CC
40	1051.5	Stretch of CC
41	1062.4	Stretch of CC
42	1069.9	Bend of 6-membered ring H
43	1077.4	Bend of 6-membered ring H
44	1112.2	Stretch of CC
45	1142.8	Stretch of CC
46	1157.4	Bend of 6-membered ring H
47	1162.3	Bend of 6-membered ring H
48	1172.7	Stretch of CC
49	1186.0	Stretch of CC
50	1189.6	Stretch of CC
51	1221.3	Stretch of CC
52	1270.9	Deformation of 5 and 6-membered rings
53	1284.0	Deformation of 5 and 6-membered rings
54	1289.9	Stretch of CC
55	1291.4	Bend of 6-membered ring H
56	1295.7	Stretch of CC
57	1299.9	Deformation of 5 and 6-membered rings

58	1305.2	Stretch of CC
59	1318.7	Stretch of CC
60	1338.8	Deformation of 5 and 6-membered rings
61	1347.9	Deformation of 5 and 6-membered rings
62	1381.7	Stretch of CC
63	1386.7	Stretch of CC
64	1395.3	Stretch of CC
65	1407.0	Stretch of CC
66	1421.1	Bend of 5-membered ring H
67	1437.1	Bend of 5-membered ring H
68	1458.6	Bend of 5-membered ring H
69	1471.0	Bend of 5-membered ring H
70	1480.7	Bend of 5-membered ring H
71	1489.9	Bend of 5-membered ring H
72	1501.9	Bend of 5-membered ring H
73	1546.6	Bend of 5-membered ring H
74	1603.2	Stretch of CC
75	1620.1	Stretch of CC
76	1635.1	Rocking of 6-membered ring H
77	1644.5	Rocking of 6-membered ring H
78	1646.4	Bend of 5-membered ring H
79	1650.1	Bend of 5-membered ring H
80	1657.0	Bend of 5-membered ring H
81	1664.0	Bend of 5-membered ring H
82	1704.7	Stretch of N_2
83	1776.8	Stretch of CC
84	1796.7	Stretch of CC
85	1806.5	Stretch of CC
86	1809.4	Stretch of CC
87	3138.3	Stretch of CH
88	3174.2	Stretch of CH
89	3182.8	Stretch of CH
90	3197.1	Stretch of CH

91	3207.5	Stretch of CH
92	3225.2	Stretch of CH
93	3243.0	Stretch of CH
94	3245.1	Stretch of CH
95	3264.9	Stretch of CH
96	3285.7	Stretch of CH
97	3355.8	Stretch of CH
98	3356.0	Stretch of CH
99	3374.8	Stretch of CH
100	3378.1	Stretch of CH
101	3394.0	Stretch of CH
102	3401.0	Stretch of CH

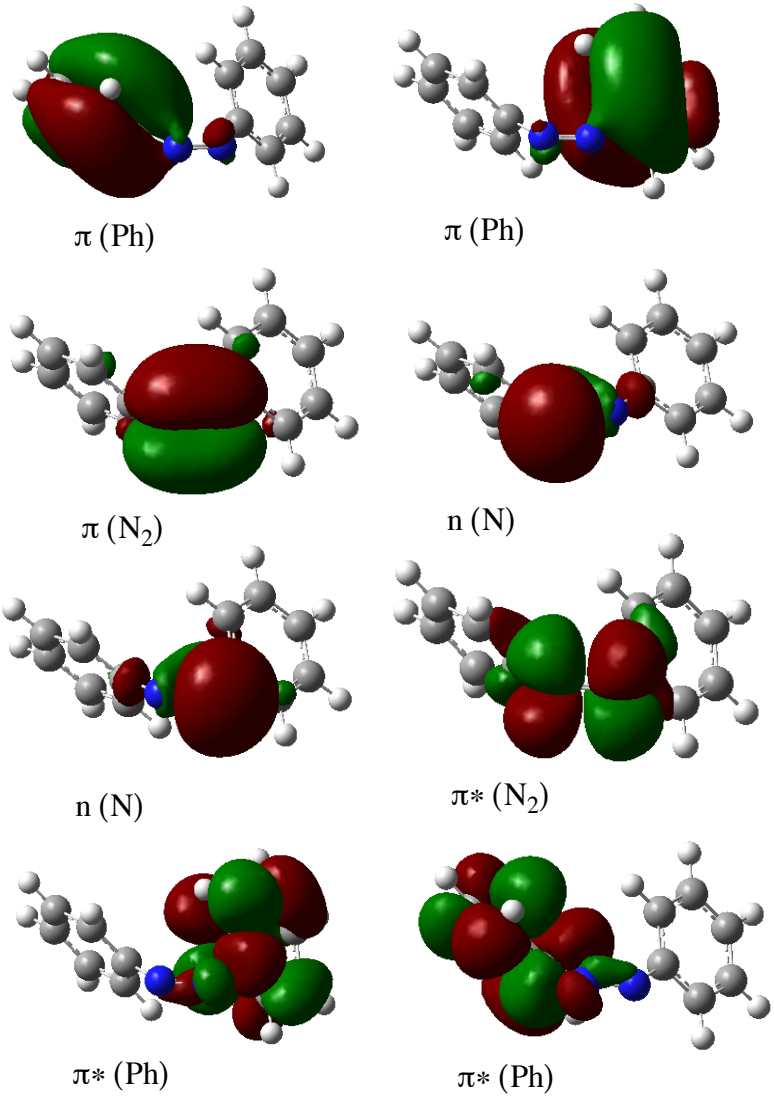

Fig. S1 Orbitals constituting the active space for the CASSCF calculations given at the equilibrium geometry with the *cis* form for azobenzene **1**; two π orbitals of the Ph groups, π orbital of the N_2, two nonbonding orbitals of the N atoms, π* orbital of the N_2 and two π* orbitals of the Ph groups for eight orbitals and the π orbital of the N_2, two nonbonding orbitals of the N atoms, π* orbital of the N_2 and one π* orbital of the Ph group for five orbitals.

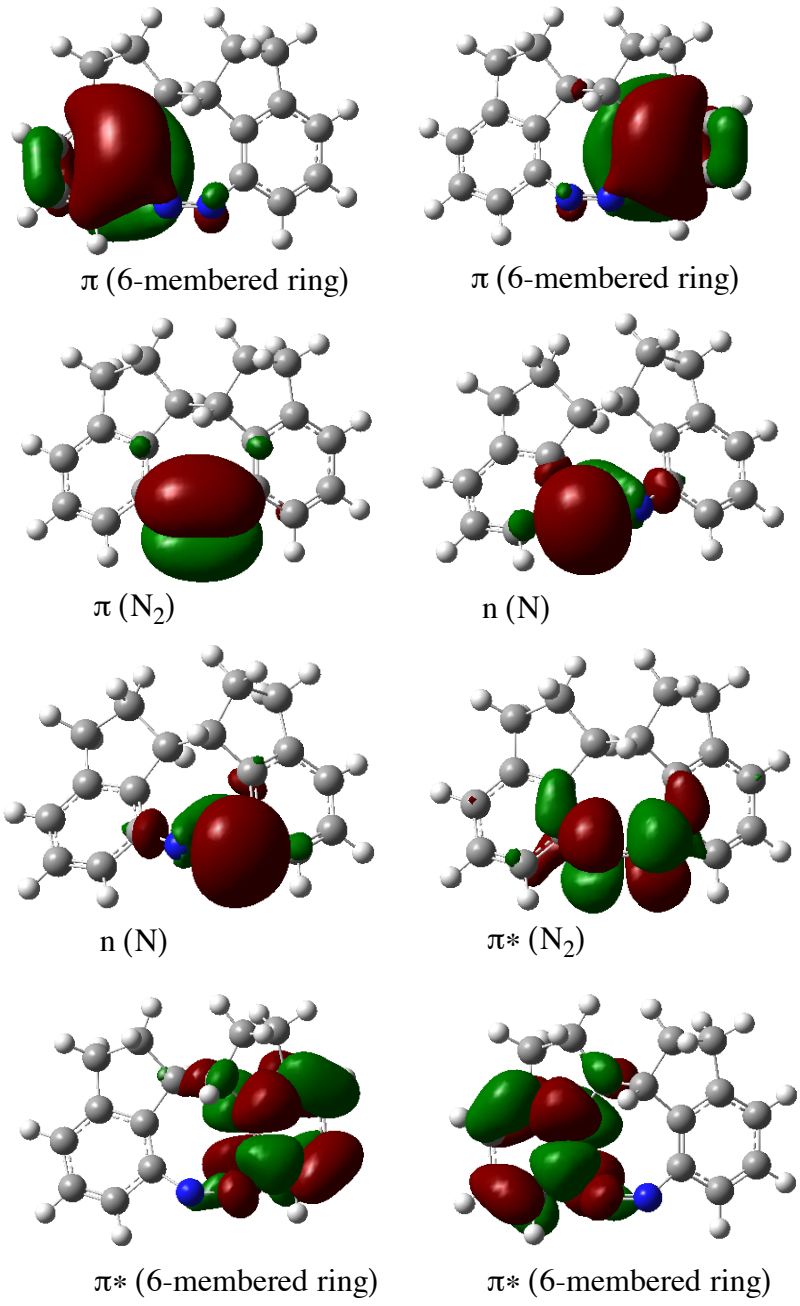

Fig. S2 Orbitals constituting the active space for the CASSCF calculations given at the equilibrium geometry with the *cis* form for diindane diazocine **4**; two π orbitals of the six-membered rings, π orbital of the N_2, two nonbonding orbitals of the N atoms, π* orbital of the N_2 and two π* orbitals of the six-membered rings for eight orbitals and the π orbital of the N_2, two nonbonding orbitals of the N atoms, π* orbital of the N_2 and one π* orbital of the six-membered ring for five orbitals.

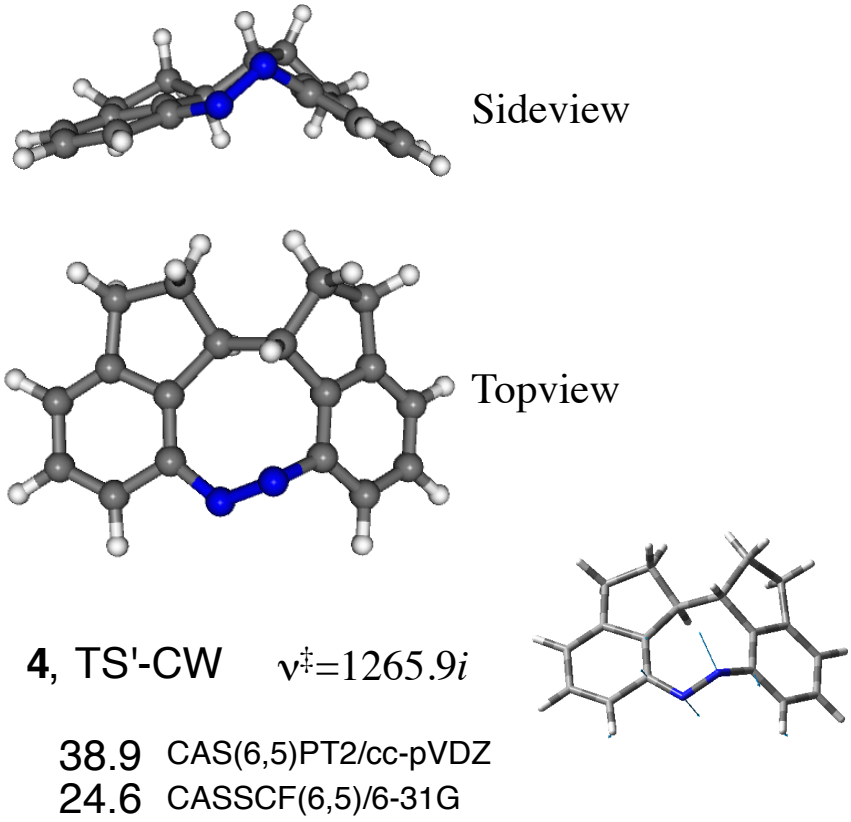

Fig. S3 Optimized structure of the transition state TS'-CW by the clockwise rotation of the –N=N– moiety in the ground state (S_0) at the CASSCF(6,5)/6-31G level for diindane diazocine **4**. The imaginary frequency (cm^{-1}), its displacement vector and energies (kcal/mol) at the CASSCF(6,5)/6-31G and CAS(6,5)PT2/cc-pVDZ levels relative to those of the *cis* form were presented together.

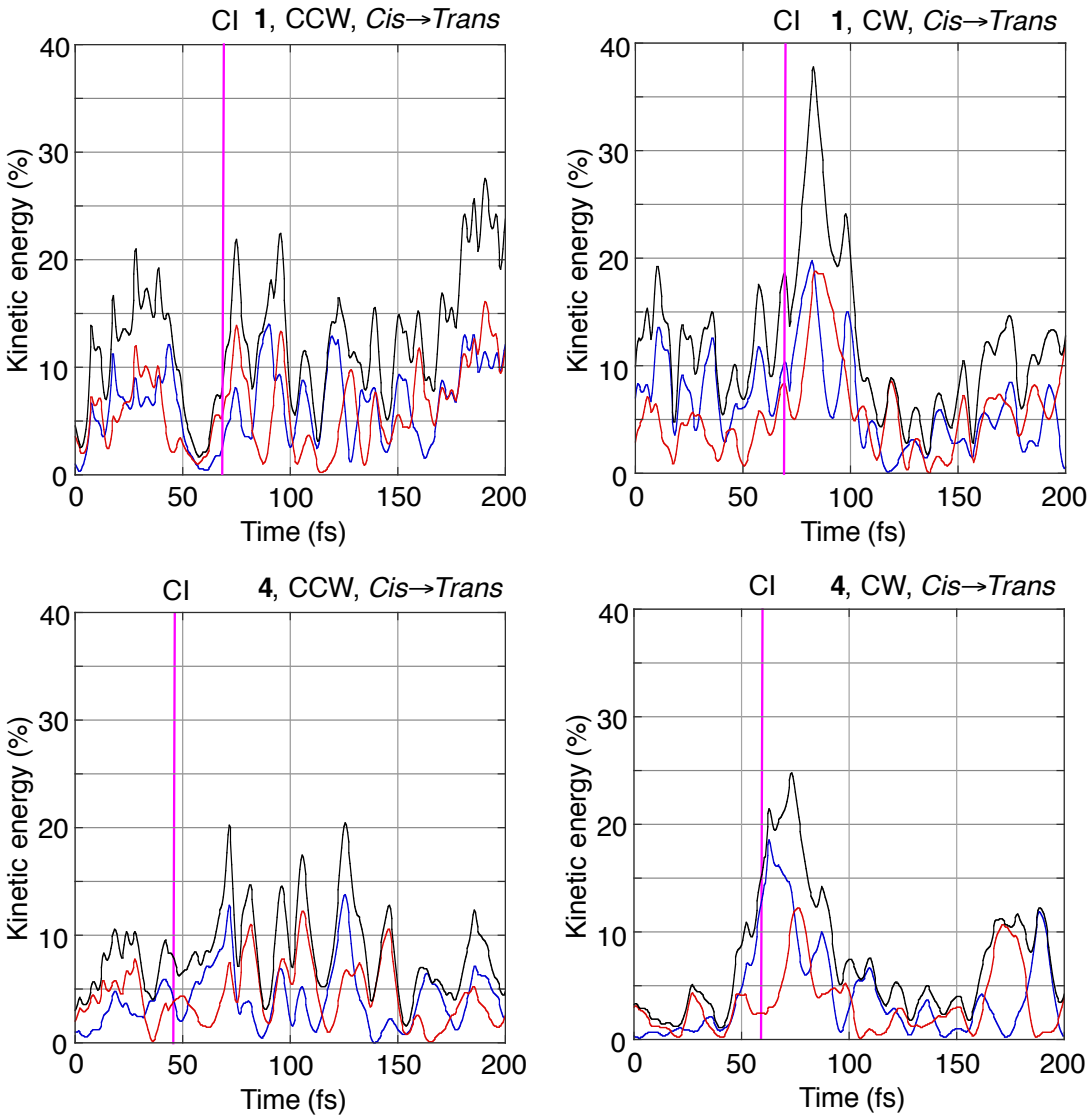

Fig. S4 Changes in the ratio of the kinetic energy of the N atoms in the isomerization of *cis*→*trans* by the clockwise (CW) and counterclockwise (CCW) rotations for azobenzene **1** and diindane diazocine **4**. Legend: N^1 [red]; N^2 [blue]; N_2 [black].

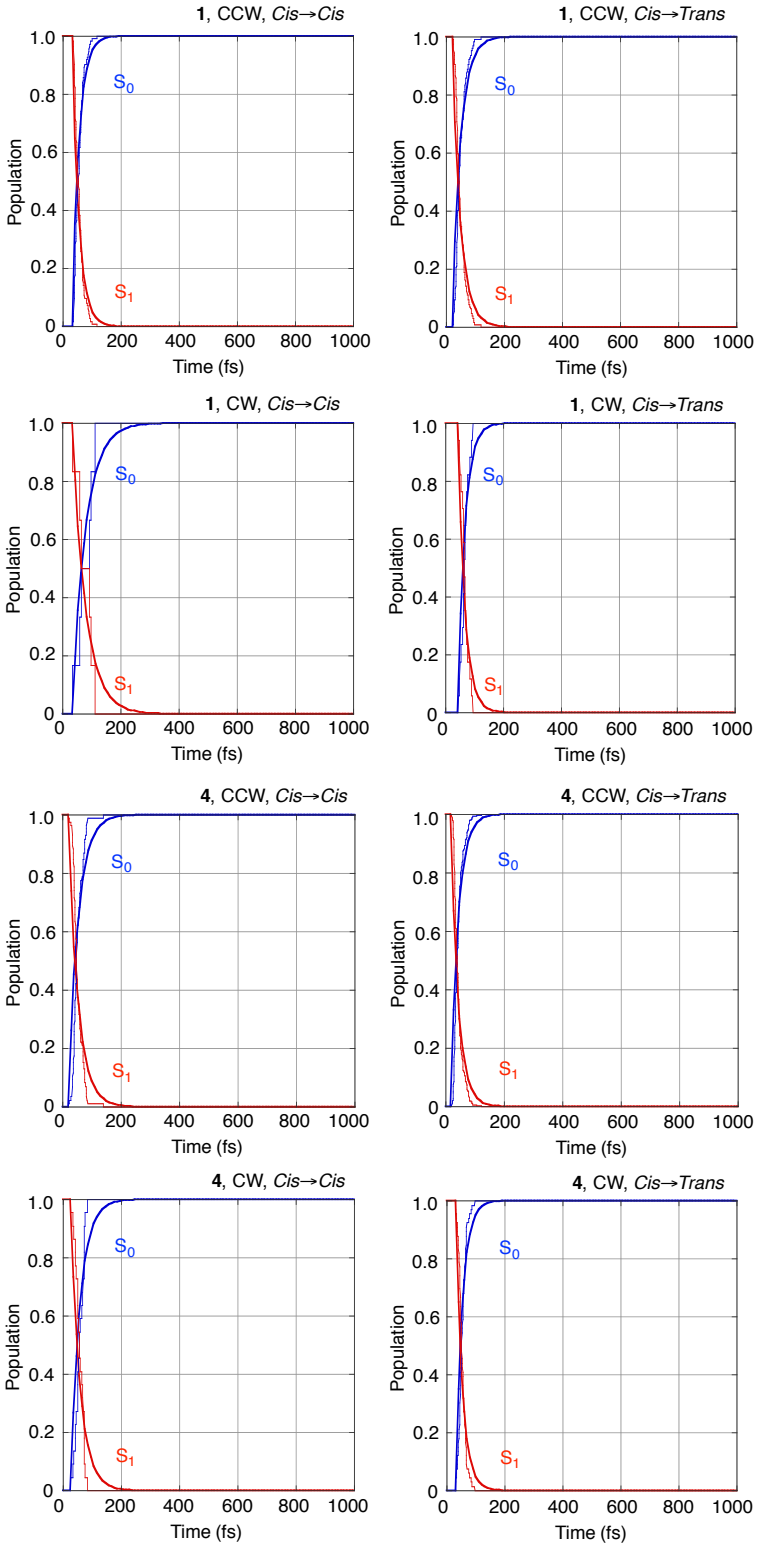

Fig. S5 Relative populations obtained from an ensemble (thin lines) and global fits (thick lines) to the populations in the reactions of *cis*→*cis* and *cis*→*trans* by both clockwise (CW) and counterclockwise (CCW) rotations after the S_1 excitation for azobenzene **1** and diindane diazocine **4**.

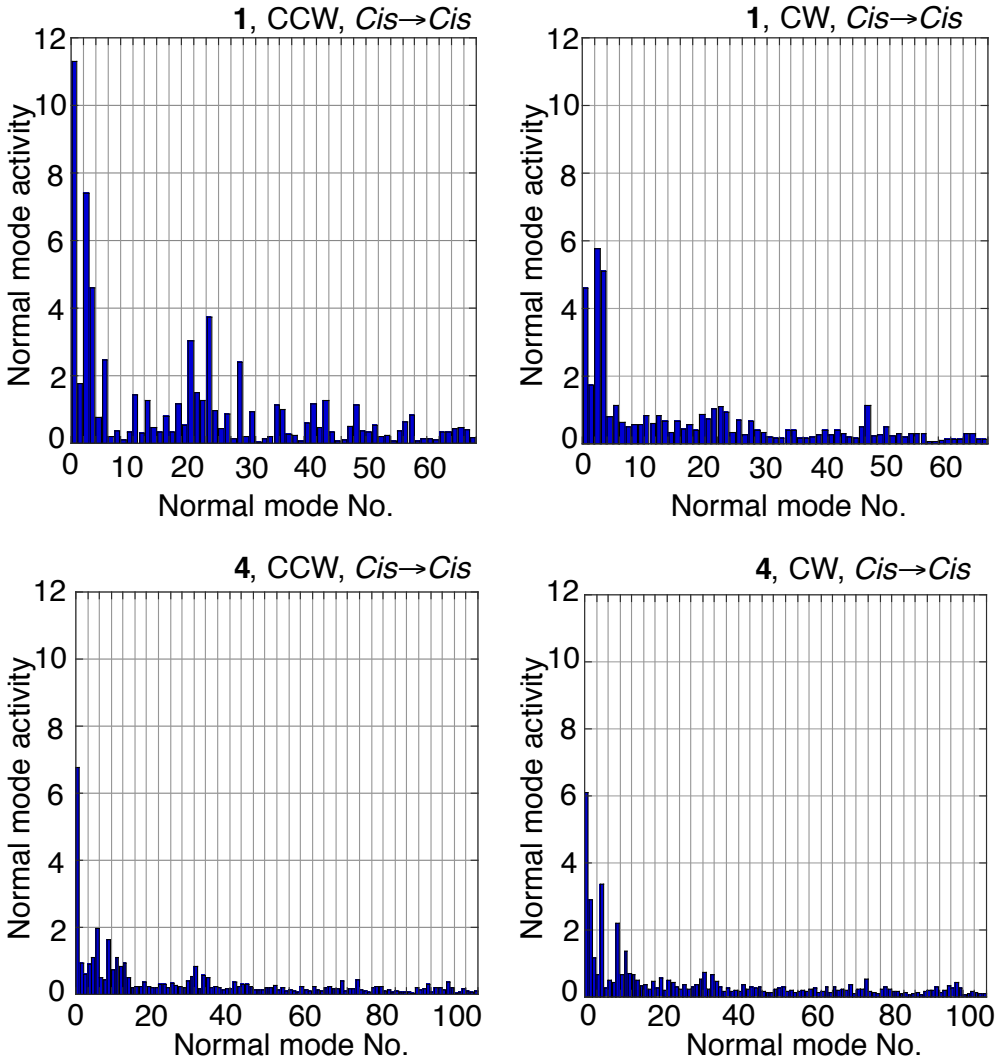

Fig. S6 Activity of all normal modes obtained from an ensemble in the reactions of *cis*→*cis* by both clockwise (CW) and counterclockwise (CCW) rotations after the internal conversion to the S_0 state (100–1000 fs) for azobenzene **1** and diindane diazocine **4**.

Cartesian coordinates (in Å)

1 (*cis*, level 1)

N	0.631811	-1.957893	0.017204
N	-0.627430	-1.961308	-0.024043
C	1.441802	-0.767429	0.099838
C	-1.442906	-0.771765	-0.094977
C	-2.488472	-0.674242	0.801911
C	-3.371452	0.415298	0.725553
C	-3.217577	1.356839	-0.261196
C	-2.175432	1.231499	-1.194579
C	-1.293283	0.184911	-1.116735
H	-2.621006	-1.438235	1.542725
H	-4.173157	0.496426	1.433604
H	-3.896651	2.184332	-0.331133
H	-2.069914	1.960635	-1.974361
H	-0.499886	0.088791	-1.830819
C	2.486274	-0.662617	-0.807385
C	3.359454	0.410710	-0.731696
C	3.212283	1.358494	0.272446
C	2.187984	1.228309	1.199079
C	1.297500	0.167899	1.114911
H	2.609806	-1.423941	-1.552449
H	4.158809	0.498054	-1.441645
H	3.895616	2.182659	0.338860
H	2.079861	1.949088	1.986114
H	0.508795	0.069171	1.833948

1 (CI-CW, level 1)

N	0.506765	1.116972	0.770549
N	-0.598311	1.505492	0.181067
C	1.627903	0.493124	0.280292
C	-1.681541	0.577447	0.139287
C	-2.810184	1.012571	-0.543745
C	-3.909545	0.178896	-0.665770
C	-3.885690	-1.085799	-0.093063
C	-2.761763	-1.513640	0.602122
C	-1.657501	-0.685300	0.721539
H	-2.805928	1.997242	-0.966969
H	-4.778793	0.513623	-1.197257
H	-4.738116	-1.731163	-0.181741
H	-2.747143	-2.487192	1.052086
H	-0.794949	-1.008045	1.268779
C	2.684197	0.213216	1.182124
C	3.817606	-0.402871	0.733343
C	3.953794	-0.760089	-0.621887
C	2.936387	-0.485209	-1.502477
C	1.763326	0.141534	-1.066474
H	2.571363	0.497751	2.209188
H	4.615032	-0.613916	1.419493
H	4.850757	-1.240954	-0.959982
H	3.032001	-0.748529	-2.538290
H	0.974676	0.360651	-1.758364

1 (*cis*, level 2)

N	-0.619108	2.035075	0.042041
N	0.598873	2.037980	-0.006232
C	-1.363185	0.804103	0.104468
C	1.347591	0.808198	-0.092451
C	2.296877	0.562494	0.897656
C	3.119397	-0.559834	0.806378
C	3.027194	-1.404413	-0.281112
C	2.109003	-1.135462	-1.298276
C	1.268688	-0.028870	-1.210549
H	2.387222	1.242597	1.722483
H	3.835131	-0.755412	1.581424
H	3.668341	-2.261614	-0.353314
H	2.049660	-1.780763	-2.153117
H	0.569035	0.183527	-1.993633
C	-2.323375	0.591144	-0.856274
C	-3.138423	-0.546242	-0.795529
C	-3.013809	-1.431920	0.248362
C	-2.068264	-1.191147	1.256001
C	-1.245178	-0.080398	1.189810
H	-2.443651	1.303627	-1.649410
H	-3.869450	-0.712357	-1.562961
H	-3.644274	-2.298188	0.302521
H	-1.982320	-1.868899	2.083072
H	-0.527145	0.110188	1.961379

1 (*trans*, level 1)

N	-0.388629	0.480109	0.000009
N	0.395269	-0.469761	-0.000047
C	1.786439	-0.177038	-0.000020
C	-1.781876	0.181674	0.000004
C	-2.636232	1.280063	0.000037
C	-4.016094	1.087051	0.000035
C	-4.536617	-0.191264	0.000003
C	-3.680760	-1.298996	-0.000029
C	-2.302176	-1.118836	-0.000030
H	-2.211149	2.264065	0.000063
H	-4.671826	1.936362	0.000060
H	-5.599715	-0.338981	0.000003
H	-4.089055	-2.291350	-0.000053
H	-1.634622	-1.955575	-0.000054
C	2.632481	-1.275821	0.000033
C	4.007581	-1.092703	0.000061
C	4.532387	0.191110	0.000027
C	3.681125	1.291729	-0.000032
C	2.308837	1.113233	-0.000055
H	2.200746	-2.256973	0.000052
H	4.661283	-1.943231	0.000106
H	5.595650	0.336740	0.000045
H	4.089071	2.284143	-0.000062
H	1.642560	1.951153	-0.000101

1 (CI-CCW, level 1)

N	-0.388629	0.480109	0.000009
N	0.395269	-0.469761	-0.000047
C	1.786439	-0.177038	-0.000020
C	-1.781876	0.181674	0.000004
C	-2.636232	1.280063	0.000037
C	-4.016094	1.087051	0.000035
C	-4.536617	-0.191264	0.000003
C	-3.680760	-1.298996	-0.000029
C	-2.302176	-1.118836	-0.000030
H	-2.211149	2.264065	0.000063
H	-4.671826	1.936362	0.000060
H	-5.599715	-0.338981	0.000003
H	-4.089055	-2.291350	-0.000053
H	-1.634622	-1.955575	-0.000054
C	2.632481	-1.275821	0.000033
C	4.007581	-1.092703	0.000061
C	4.532387	0.191110	0.000027
C	3.681125	1.291729	-0.000032
C	2.308837	1.113233	-0.000055
H	2.200746	-2.256973	0.000052
H	4.661283	-1.943231	0.000106
H	5.595650	0.336740	0.000045
H	4.089071	2.284143	-0.000062
H	1.642560	1.951153	-0.000101

1 (*trans*, level 2)

N	0.371160	-0.481280	0.000079
N	-0.372044	0.484552	0.000117
C	-1.761568	0.186576	0.000051
C	1.762273	-0.183162	0.000019
C	2.605905	-1.273521	0.000742
C	3.991305	-1.097305	0.000742
C	4.524192	0.187629	-0.000042
C	3.666368	1.297079	-0.000813
C	2.289246	1.119073	-0.000776
H	2.177388	-2.256442	0.001323
H	4.638571	-1.952639	0.001333
H	5.587626	0.331068	-0.000085
H	4.075229	2.289222	-0.001439
H	1.625031	1.957618	-0.001346
C	-2.606579	1.270992	0.000778
C	-3.996486	1.087357	0.000750
C	-4.520201	-0.181667	-0.000044
C	-3.661058	-1.296042	-0.000813
C	-2.291092	-1.119919	-0.000760
H	-2.184186	2.256447	0.001376
H	-4.644111	1.942440	0.001341
H	-5.583176	-0.328536	-0.000092
H	-4.073545	-2.286490	-0.001446
H	-1.626489	-1.958129	-0.001328

1 (CI-CW, level 2)

N	0.484624	-1.139007	-0.724487
N	-0.593621	-1.496790	-0.123620
C	1.613206	-0.503408	-0.259457
C	-1.656136	-0.580236	-0.119856
C	-2.825796	-1.012842	0.539517
C	-3.912690	-0.183826	0.628930
C	-3.870768	1.096606	0.053400
C	-2.738627	1.522570	-0.604193
C	-1.620737	0.689772	-0.700015
H	-2.835726	-1.997233	0.964139
H	-4.800180	-0.511629	1.134262
H	-4.727051	1.739128	0.123256
H	-2.709710	2.497768	-1.050287
H	-0.746471	1.016607	-1.224665
C	2.663492	-0.257637	-1.177389
C	3.812416	0.372802	-0.750186
C	3.951103	0.770494	0.593662
C	2.930232	0.523766	1.476589
C	1.752899	-0.113442	1.060119
H	2.545989	-0.572652	-2.195222
H	4.607035	0.558070	-1.447086
H	4.848706	1.258639	0.919319
H	3.023164	0.817539	2.504642
H	0.965659	-0.303377	1.761663

1 (CI-CCW, level 2)

N	-0.485924	-1.108218	-0.760617
N	0.581186	-1.488350	-0.173042
C	1.670755	-0.580770	-0.131621
C	2.800229	-1.025320	0.515871
C	3.919725	-0.191134	0.636279
C	3.897234	1.071683	0.097657
C	2.749449	1.528593	-0.576730
C	1.641397	0.713542	-0.694764
H	4.753736	1.712051	0.183534
H	2.737864	2.512908	-1.003045
H	0.768197	1.048684	-1.215944
C	-1.619481	-0.490521	-0.274144
C	-1.760093	-0.145229	1.056747
C	-2.938641	0.476524	1.493347
C	-3.958353	0.751631	0.617605
C	-3.817959	0.399191	-0.738659
C	-2.667913	-0.216096	-1.184830
H	-4.856913	1.227678	0.958242
H	-4.612052	0.606772	-1.429810
H	-2.548918	-0.497761	-2.212216
H	-3.033183	0.735765	2.530470
H	-0.973157	-0.358583	1.751862
H	2.806803	-2.016424	0.924653
H	4.792688	-0.547669	1.147315

1 (*cis*, level 3)

N	0.617475	2.033329	-0.039966
N	-0.599669	2.035111	0.007645
C	1.364353	0.805448	-0.103587
C	-1.349180	0.807695	0.094110
C	-2.296391	0.561174	-0.898191
C	-3.115142	-0.560445	-0.811003
C	-3.026390	-1.407099	0.279355
C	-2.113434	-1.134331	1.297957
C	-1.272794	-0.026986	1.211243
H	-2.381513	1.245805	-1.731037
H	-3.833380	-0.758926	-1.595436
H	-3.672616	-2.271770	0.349727
H	-2.054393	-1.782687	2.161656
H	-0.571618	0.188480	2.003756
C	2.320147	0.589826	0.859805
C	3.133675	-0.550658	0.799787
C	3.014347	-1.432121	-0.247613
C	2.075271	-1.184278	-1.260086
C	1.251378	-0.074040	-1.193245
H	2.433828	1.304690	1.663470
H	3.865633	-0.722529	1.577660
H	3.649721	-2.305897	-0.301536
H	1.991649	-1.862937	-2.098139
H	0.532995	0.121582	-1.975067

1 (*trans*, level 3)

N	0.371853	-0.478403	0.000132
N	-0.373107	0.485199	0.000142
C	-1.761991	0.187018	0.000130
C	1.762583	-0.180676	0.000128
C	2.606768	-1.273378	0.000048
C	3.990571	-1.098099	-0.000106
C	4.524703	0.186549	-0.000180
C	3.668292	1.295293	-0.000076
C	2.290411	1.119555	0.000082
H	2.172128	-2.263167	0.000075
H	4.642624	-1.960991	-0.000189
H	5.597049	0.329889	-0.000322
H	4.080540	2.295575	-0.000140
H	1.621185	1.965074	0.000129
C	-2.606266	1.270353	0.000060
C	-3.998822	1.086423	-0.000091
C	-4.521489	-0.181682	-0.000163
C	-3.660816	-1.296440	-0.000078
C	-2.291325	-1.120897	0.000068
H	-2.178890	2.263214	0.000088
H	-4.652015	1.948595	-0.000165
H	-5.593366	-0.329769	-0.000294
H	-4.076093	-2.295335	-0.000144
H	-1.620090	-1.964764	0.000107

1 (CI-CW, level 3)

N	0.487727	-1.139003	-0.728448
N	-0.592574	-1.489537	-0.123918
C	1.612825	-0.503688	-0.258398
C	-1.652877	-0.579141	-0.120392
C	-2.819221	-1.011714	0.547340
C	-3.907956	-0.185750	0.637667
C	-3.873522	1.091678	0.052851
C	-2.744936	1.516587	-0.614041
C	-1.625406	0.689369	-0.709850
H	-2.821926	-2.001072	0.982437
H	-4.798303	-0.517146	1.154732
H	-4.738156	1.738038	0.122131
H	-2.722424	2.496887	-1.070893
H	-0.748097	1.019019	-1.245285
C	2.667261	-0.263089	-1.175301
C	3.814314	0.368111	-0.747047
C	3.950554	0.772389	0.597167
C	2.926964	0.530039	1.476017
C	1.747305	-0.108483	1.058948
H	2.550771	-0.584830	-2.200261
H	4.616906	0.550537	-1.449320
H	4.854732	1.264972	0.927177
H	3.017742	0.830806	2.511690
H	0.950865	-0.295278	1.764387

1 (CI-CCW, level 3)

N	-0.490146	-1.093351	-0.788895
N	0.577745	-1.478168	-0.203559
C	1.668053	-0.577316	-0.143596
C	2.789411	-1.032662	0.508713
C	3.912901	-0.202839	0.646650
C	3.901034	1.063592	0.119063
C	2.759851	1.531147	-0.561820
C	1.648916	0.723711	-0.696006
H	4.767162	1.704121	0.218579
H	2.755494	2.526994	-0.983871
H	0.775391	1.071587	-1.226086
C	-1.619842	-0.485053	-0.283346
C	-1.755190	-0.164681	1.052806
C	-2.935358	0.450322	1.503621
C	-3.956644	0.742151	0.637485
C	-3.818709	0.413841	-0.727222
C	-2.671286	-0.193774	-1.187543
H	-4.861307	1.215992	0.992817
H	-4.620245	0.635912	-1.419175
H	-2.552806	-0.458737	-2.228411
H	-3.027952	0.692700	2.554298
H	-0.959805	-0.392501	1.747324
H	2.785079	-2.035385	0.912087
H	4.786971	-0.570679	1.166770

1 (TS, level 1)

N	0.443739	-0.977652	0.009657
N	-0.697976	-1.457738	0.012702
C	1.693489	-0.452109	0.004362
C	-1.818193	-0.532265	0.005311
C	-3.067467	-1.115850	0.005052
C	-4.214296	-0.302784	-0.002518
C	-4.082313	1.062476	-0.009348
C	-2.803808	1.650905	-0.008763
C	-1.680026	0.867724	-0.001587
H	-3.142360	-2.185216	0.010492
H	-5.186620	-0.755338	-0.002910
H	-4.952876	1.689518	-0.015152
H	-2.712705	2.719850	-0.014026
H	-0.703175	1.308895	-0.001177
C	2.342432	-0.193979	-1.210124
C	3.618267	0.341034	-1.198576
C	4.270067	0.628066	-0.006959
C	3.618172	0.366285	1.190388
C	2.342206	-0.168140	1.213164
H	1.848152	-0.418174	-2.134032
H	4.105860	0.532778	-2.135397
H	5.258829	1.041616	-0.011298
H	4.105661	0.577911	2.122972
H	1.847720	-0.372299	2.141601

4 (*cis*, level 1)

N	-0.627160	-2.067322	1.048845
N	0.595856	-2.175946	0.993466
C	1.525810	-1.405983	0.236125
C	1.647126	-0.047272	0.316533
C	0.718371	0.959547	0.960476
C	-0.458368	1.182992	-0.005921
C	-1.532688	0.099389	-0.032076
C	-1.560881	-1.229284	0.332307
C	2.501016	-2.150593	-0.459215
C	3.534836	-1.517764	-1.094762
C	3.668784	-0.115866	-1.017691
C	2.734552	0.602986	-0.303578
C	-2.763699	-1.961705	0.149489
C	-3.881339	-1.400587	-0.390676
C	-3.880415	-0.028200	-0.715721
C	-2.733426	0.697657	-0.512818
C	1.648073	2.192860	1.114987
H	-0.039173	1.220819	-1.011409
H	2.417563	-3.219270	-0.462579
H	4.264360	-2.092984	-1.631243
H	4.498930	0.372248	-1.492372
C	2.663844	2.092787	-0.045817
H	-2.760958	-2.980708	0.479067
H	-4.770079	-1.986051	-0.523195
H	-4.773463	0.444510	-1.078979
C	-2.548310	2.189204	-0.684580
C	-1.295042	2.469457	0.164251
H	-3.413875	2.753993	-0.361663
H	-2.363861	2.442817	-1.725871
H	-1.569056	2.602437	1.206886
H	-0.764827	3.354092	-0.161486
H	2.175619	2.107303	2.058766
H	1.113170	3.131386	1.128320
H	2.308953	2.621623	-0.926611
H	3.625595	2.517891	0.214408
H	0.340777	0.635031	1.923899

4 (*trans*-CW, level 1)

N	0.347333	-1.736401	-0.509705
N	-0.348108	-1.736885	0.508897
C	-1.694205	-1.331532	0.276648
C	-1.777620	-0.007793	-0.126130
C	-0.648359	0.995225	-0.440004
C	0.648393	0.995734	0.439089
C	1.776229	-0.009313	0.126903
C	1.692685	-1.329396	-0.277212
C	-2.841401	-2.065222	0.588920
C	-4.072908	-1.472238	0.428549
C	-4.180977	-0.140029	-0.003645
C	-3.041753	0.581758	-0.266042
C	2.842591	-2.065367	-0.590203
C	4.071856	-1.473762	-0.428313
C	4.180597	-0.139725	0.006354
C	3.044066	0.581396	0.268595
C	-1.429930	2.339764	-0.330670
H	0.345566	0.855091	1.474237
H	-2.752324	-3.074315	0.939962
H	-4.963187	-2.029417	0.648127
H	-5.151184	0.307969	-0.108314
C	-2.892669	2.018868	-0.703599
H	2.752068	-3.073506	-0.943407
H	4.962525	-2.030248	-0.648169
H	5.151436	0.306920	0.111282
C	2.892671	2.018346	0.705643
C	1.431381	2.339191	0.326998
H	3.599419	2.684860	0.226300
H	3.041362	2.106585	1.779043
H	1.402435	2.681113	-0.702961
H	1.007066	3.117597	0.946226
H	-1.006769	3.115619	-0.953889
H	-1.397800	2.685333	0.697932
H	-3.597670	2.684947	-0.221063
H	-3.046444	2.106811	-1.776254
H	-0.344965	0.852203	-1.474685

4 (*trans*-CCW, level 1)

N	-0.357381	-1.734189	-0.510806
N	0.378713	-1.776559	0.472565
C	1.714035	-1.361681	0.196048
C	1.796701	0.024997	0.108897
C	0.696159	1.081324	0.349011
C	-0.708565	1.086589	-0.364080
C	-1.801370	0.027884	-0.121788
C	-1.702478	-1.360702	-0.214914
C	2.832648	-2.163545	0.111216
C	4.073598	-1.564572	-0.080267
C	4.187062	-0.183584	-0.146406
C	3.048496	0.604053	-0.035232
C	-2.816659	-2.180960	-0.104639
C	-4.063490	-1.586869	0.107219
C	-4.183904	-0.196367	0.171429
C	-3.060344	0.597888	0.043001
C	1.451725	2.390577	-0.055242
H	-0.514381	1.101297	-1.435035
H	2.739598	-3.228821	0.187019
H	4.949448	-2.178496	-0.164613
H	5.152196	0.271648	-0.265645
C	2.963647	2.106965	0.042602
H	-2.715701	-3.245887	-0.176919
H	-4.934834	-2.204430	0.208901
H	-5.152032	0.249162	0.304489
C	-2.979195	2.102411	-0.033115
C	-1.466305	2.391139	0.053557
H	-3.532595	2.596806	0.756865
H	-3.391536	2.449237	-0.976653
H	-1.209059	2.624430	1.081446
H	-1.180387	3.239377	-0.552784
H	1.157172	3.234025	0.553498
H	1.201390	2.628048	-1.083826
H	3.522429	2.603336	-0.742487
H	3.368887	2.453380	0.989567
H	0.499521	1.088834	1.420087

4 (CI-CW, level 1)

N	0.466914	-2.217351	0.190256
N	-0.553380	-1.876659	1.001603
C	1.611080	-1.429626	-0.029074
C	2.698276	-2.082385	-0.609954
C	1.705720	-0.075089	0.271273
C	3.863598	-1.392247	-0.889021
C	2.877687	0.611676	-0.032462
C	3.959452	-0.034450	-0.604195
C	-1.687637	-1.224425	0.400464
C	-2.895075	-1.914846	0.451798
C	-1.655421	0.069749	-0.093710
C	-4.058831	-1.327342	-0.012049
C	-2.844697	0.669543	-0.508743
C	-4.040905	-0.020891	-0.489538
C	0.638187	0.860487	0.822934

C	-0.496902	1.055736	-0.218568
H	-0.061014	0.940119	-1.209780
C	-1.249372	2.409863	-0.202017
H	2.606608	-3.127182	-0.828253
H	4.693848	-1.909079	-1.329756
H	4.860136	0.504038	-0.831198
H	-2.905804	-2.902470	0.868119
H	-4.981037	-1.874035	0.024881
H	-4.949865	0.449447	-0.814079
C	1.470423	2.128999	1.172313
H	0.195634	0.469606	1.731624
C	2.741936	2.078752	0.299452
H	0.917409	3.047563	1.045930
H	1.754313	2.068594	2.216982
H	3.607915	2.472777	0.818416
H	2.623545	2.662738	-0.609807
C	-2.594398	2.109395	-0.896158
H	-1.433060	2.716208	0.823219
H	-0.693925	3.197472	-0.694280
H	-3.387526	2.774278	-0.576622
H	-2.500639	2.210603	-1.974877

4 (CI-CCW, level 1)

N	-0.502685	-2.203296	0.196920
N	0.577763	-2.012732	0.985247
C	1.686410	-1.366214	0.341866
C	1.728536	0.008955	0.291612
C	0.684763	0.990125	0.789013
C	-0.527619	1.107456	-0.172900
C	-1.643220	0.045486	-0.083949
C	-1.627597	-1.346309	0.053193
C	2.744330	-2.117617	-0.151109
C	3.835196	-1.473641	-0.715341
C	3.888140	-0.084070	-0.771189
C	2.834352	0.649566	-0.256132
C	-2.828322	-2.059537	0.001966
C	-4.040510	-1.421965	-0.164541
C	-4.071815	-0.042786	-0.306961
C	-2.885777	0.664058	-0.274382
C	1.542480	2.290573	0.892253
H	-0.144380	1.089408	-1.192510
H	2.709881	-3.186929	-0.084748
H	4.650641	-2.055307	-1.099734
H	4.743835	0.406348	-1.195397
C	2.664616	2.147817	-0.160330
H	-2.776157	-3.124582	0.100433
H	-4.947452	-1.993852	-0.188212
H	-5.003950	0.470755	-0.448678
C	-2.738807	2.150451	-0.473295
C	-1.319169	2.426458	0.033213
H	-3.490188	2.721103	0.059334
H	-2.832471	2.400841	-1.527230
H	-1.350394	2.659809	1.093100
H	-0.856985	3.260796	-0.475987
H	1.990909	2.316063	1.879550
H	0.974074	3.199620	0.775565
H	2.366068	2.566156	-1.118457
H	3.573446	2.655472	0.139987
H	0.311654	0.713662	1.769885

4 (*cis*, level 2)

N	-0.635533	-1.989853	1.205161
N	0.569783	-2.113098	1.156069
C	1.457931	-1.413655	0.286686
C	1.638090	-0.041992	0.342969
C	0.755026	1.004513	0.992666
C	-0.437825	1.220124	0.049539
C	-1.497927	0.122266	0.001891
C	-1.521733	-1.205744	0.375121
C	2.357260	-2.191532	-0.458480
C	3.374034	-1.595915	-1.167652
C	3.566579	-0.207248	-1.114577
C	2.700449	0.558625	-0.349179
C	-2.697196	-1.958976	0.122961
C	-3.792636	-1.417570	-0.484451
C	-3.803501	-0.046106	-0.800490
C	-2.680817	0.700983	-0.533231
C	1.716580	2.220885	1.067544
H	-0.025399	1.269820	-0.959221
H	2.244624	-3.258165	-0.453070
H	4.043609	-2.203228	-1.745744
H	4.380712	0.245249	-1.648598
C	2.690228	2.056139	-0.123918
H	-2.704283	-2.978021	0.455193
H	-4.659636	-2.021360	-0.669849
H	-4.686467	0.411658	-1.205111
C	-2.516526	2.198897	-0.678205
C	-1.296902	2.490618	0.217799
H	-3.403615	2.742480	-0.377832
H	-2.300335	2.472338	-1.708425
H	-1.606292	2.601800	1.253017
H	-0.773264	3.389598	-0.078154
H	2.274772	2.160388	1.995538
H	1.202408	3.171389	1.061839
H	2.327668	2.577323	-1.005793
H	3.674402	2.451810	0.096699
H	0.404660	0.721699	1.978942

4 (*trans*-CW, level 2)

N	-0.321475	-1.708198	0.526347
N	0.323336	-1.723557	-0.506946
C	1.671852	-1.330730	-0.274240
C	1.770743	-0.004585	0.120944
C	0.652473	1.008845	0.438052
C	-0.650329	1.008483	-0.428458
C	-1.773730	0.003486	-0.106866
C	-1.674089	-1.330497	0.288825
C	2.815643	-2.074294	-0.582527
C	4.052642	-1.491997	-0.424724
C	4.172884	-0.157786	-0.002279
C	3.039799	0.575406	0.255832
C	-2.814133	-2.078147	0.575422
C	-4.066997	-1.488120	0.404507
C	-4.176388	-0.156126	-0.011714
C	-3.035465	0.578923	-0.255328
C	1.441734	2.346906	0.314265
H	-0.354231	0.864335	-1.465693
H	2.719889	-3.085108	-0.927577
H	4.937974	-2.058765	-0.640240
H	5.147121	0.282372	0.098691
C	2.903720	2.017092	0.683396
H	-2.723742	-3.091541	0.914565
H	-4.953369	-2.058098	0.606064
H	-5.147491	0.288351	-0.125454
C	-2.898515	2.020824	-0.685678
C	-1.435660	2.349928	-0.318219
H	-3.604906	2.679037	-0.194178
H	-3.059399	2.115743	-1.756644
H	-1.400539	2.696772	0.709981
H	-1.017696	3.126721	-0.944040
H	1.026887	3.130644	0.933389
H	1.406786	2.684636	-0.716974
H	3.612277	2.673877	0.193285
H	3.062376	2.111954	1.754816
H	0.357931	0.875691	1.476947

4 (*trans*-CCW, level 2)

N	0.337794	-1.716128	0.511866
N	-0.344021	-1.748599	-0.492968
C	-1.684984	-1.361625	-0.208339
C	-1.789539	0.034233	-0.119918
C	-0.693779	1.094340	-0.357056
C	0.704038	1.095910	0.367696
C	1.796805	0.036675	0.126971
C	1.684546	-1.362634	0.219650
C	-2.799610	-2.177966	-0.116030
C	-4.054365	-1.585600	0.088267
C	-4.176370	-0.199992	0.155798
C	-3.035362	0.599628	0.034474
C	2.775171	-2.178896	0.116891
C	4.038785	-1.597462	-0.102000
C	4.176246	-0.221059	-0.174349
C	3.039016	0.593425	-0.042359
C	-1.455981	2.400768	0.044646
H	0.498447	1.106226	1.436876
H	-2.698562	-3.242851	-0.192206

H -4.924696 -2.206538 0.179777
H -5.142593 0.250455 0.284772
C -2.966973 2.104152 -0.038702
H 2.668579 -3.242816 0.196973
H 4.899598 -2.230561 -0.199107
H 5.145031 0.220123 -0.315068
C 2.979382 2.097650 0.026434
C 1.467814 2.401583 -0.036385
H 3.524855 2.579739 -0.777072
H 3.415364 2.445739 0.959225
H 1.200945 2.655701 -1.056579
H 1.196199 3.241334 0.588249
H -1.172637 3.242776 -0.571644
H -1.199890 2.647282 1.069610
H -3.521120 2.591880 0.755289
H -3.386661 2.451519 -0.979057
H -0.488316 1.104291 -1.426457

4 (CI-CW, level 2)
N 0.432500 -2.143103 0.086345
N -0.572258 -1.969128 0.892825
C 1.604800 -1.415452 -0.068027
C 2.702625 -2.074412 -0.626538
C 1.718960 -0.069768 0.269452
C 3.888971 -1.396676 -0.844323
C 2.910292 0.602210 0.025400
C 4.002596 -0.048886 -0.522719
C -1.692950 -1.247476 0.381674
C -2.931854 -1.898994 0.507832
C -1.652900 0.054432 -0.121635
C -4.103229 -1.281201 0.090408
C -2.854585 0.674247 -0.499710
C -4.061193 0.022904 -0.417828
C 0.636942 0.858026 0.791290
C -0.487800 1.033265 -0.267972
H -0.044569 0.897748 -1.252603
C -1.228606 2.394823 -0.269819
H 2.606676 -3.112098 -0.875909
H 4.724778 -1.919355 -1.267935
H 4.920069 0.477528 -0.705924
H -2.948391 -2.883078 0.933027
H -5.040586 -1.795171 0.179113
H -4.968906 0.514607 -0.713719
C 1.452575 2.134402 1.161030
H 0.179606 0.466820 1.693685
C 2.778937 2.065915 0.372376
H 0.913721 3.051262 0.976353
H 1.667643 2.101257 2.223058
H 3.615895 2.434631 0.954086
H 2.734648 2.664757 -0.533617
C -2.589961 2.099435 -0.928417
H -1.389498 2.725655 0.751601
H -0.672510 3.165328 -0.787820
H -3.365674 2.785617 -0.611402
H -2.516310 2.169347 -2.011033

4 (CI-CCW, level 2)
N -0.464271 -2.103533 0.275608
N 0.580700 -1.972188 1.004074
C 1.696069 -1.364705 0.349996
C 1.724288 0.007731 0.272254
C 0.688083 0.996005 0.781944
C -0.552304 1.114802 -0.142684
C -1.654225 0.042237 -0.053637
C -1.610028 -1.349241 0.083281
C 2.781565 -2.122059 -0.126573
C 3.850528 -1.479448 -0.699156
C 3.886212 -0.075048 -0.790019
C 2.835579 0.654117 -0.298024
C -2.813731 -2.095947 -0.031813
C -4.011246 -1.477870 -0.240259
C -4.071402 -0.077718 -0.355923
C -2.915778 0.647655 -0.268634
C 1.548417 2.297575 0.856025
H -0.195753 1.118772 -1.172672
H 2.759330 -3.190243 -0.036739
H 4.677563 -2.052916 -1.071509
H 4.739916 0.409481 -1.225052
C 2.644847 2.150983 -0.223223
H -2.749376 -3.160689 0.069866
H -4.909758 -2.060203 -0.308966
H -5.013371 0.410549 -0.520021
C -2.772931 2.140105 -0.430795
C -1.359437 2.418567 0.098360
H -3.535343 2.694319 0.103423
H -2.852612 2.413702 -1.480061
H -1.399925 2.619564 1.164915
H -0.907033 3.274461 -0.382968
H 2.021442 2.330854 1.831745
H 0.975753 3.205119 0.747510
H 2.311269 2.545851 -1.179725
H 3.553239 2.678724 0.041161
H 0.342613 0.726256 1.774600

4 (TS-CW, level 1)
N -0.364087 -1.799646 0.289123
N 0.755135 -2.347362 0.393903
C 1.839402 -1.421395 0.120757
C 1.718894 -0.034590 0.208489
C 0.566043 0.851688 0.716272
C -0.632027 1.048444 -0.275361
C -1.755272 0.030705 -0.147281
C -1.638909 -1.324126 0.127949
C 3.037350 -1.998977 -0.272307
C 4.118769 -1.207560 -0.625025
C 4.010823 0.174860 -0.562042
C 2.822933 0.745369 -0.134234
C -2.804425 -2.114629 0.225577
C -4.034495 -1.534827 0.035353
C -4.148006 -0.159858 -0.244592
C -3.015077 0.611922 -0.328801
C 1.335685 2.170391 1.040445
H -0.242842 1.009174 -1.290471
H 3.097368 -3.069114 -0.305216
H 5.037666 -1.663772 -0.939056
H 4.847805 0.795639 -0.821766
C 2.532835 2.211541 0.075392
H -2.706294 -3.158653 0.447097
H -4.923007 -2.131968 0.106580
H -5.120644 0.273932 -0.383334
C -2.858577 2.089091 -0.604175
C -1.425811 2.378210 -0.099360
H -3.602237 2.697260 -0.103407
H -2.941702 2.289235 -1.669510
H -1.471713 2.632099 0.954735
H -0.966481 3.207785 -0.620271
H 1.709337 2.100891 2.056747
H 0.722675 3.056011 0.985559
H 2.270390 2.695037 -0.862899
H 3.376955 2.751288 0.487946
H 0.154590 0.446662 1.633753

4 (TS'-CW, level 1)
N -0.565147 -2.224857 0.461504
N 0.508033 -1.800929 1.201684
C 1.622001 -1.337211 0.432224
C 1.742096 0.026766 0.309799
C 0.768678 1.063190 0.823201
C -0.500683 1.151764 -0.059356
C -1.599437 0.056122 0.000111
C -1.596775 -1.347186 0.133774
C 2.582887 -2.176861 -0.110727
C 3.664444 -1.618566 -0.779901
C 3.795005 -0.238185 -0.905705
C 2.826150 0.582347 -0.352178
C -2.813119 -2.062298 -0.096667
C -3.979619 -1.428311 -0.378030
C -4.000374 -0.021775 -0.471379
C -2.844989 0.680090 -0.298380
C 1.663494 2.342995 0.773453
H -0.166131 1.172209 -1.097425
H 2.491034 -3.239519 -0.003829
H 4.412703 -2.263594 -1.198531
H 4.642222 0.177170 -1.417878
C 2.724617 2.090487 -0.326073
H -2.762511 -3.128533 -0.010808

H	-4.881054	-1.990765	-0.524329
H	-4.919432	0.489685	-0.687800
C	-2.695358	2.175213	-0.419509
C	-1.319746	2.440475	0.198532
H	-3.491855	2.714285	0.078945
H	-2.709127	2.474163	-1.464932
H	-1.413128	2.596376	1.269440
H	-0.848434	3.315332	-0.225299
H	2.166224	2.434326	1.730015
H	1.112319	3.256513	0.614410
H	2.397187	2.472409	-1.289730
H	3.668124	2.571734	-0.097332
H	0.466027	0.854365	1.843626

4 (TS-CCW, level 1)

N	-0.400711	-1.887022	-0.023967
N	0.681017	-2.181983	-0.570066
C	-1.645376	-1.353752	0.146058
C	-2.741204	-2.095069	0.591749
C	-1.804996	-0.014935	-0.185982
C	-3.985218	-1.490399	0.666321
C	-3.071508	0.550282	-0.180802
C	-4.169142	-0.173264	0.254113
C	1.803106	-1.317473	-0.279740
C	3.052093	-1.941886	-0.464066
C	1.727074	0.019034	0.088302
C	4.216065	-1.261000	-0.239508
C	2.951258	0.696083	0.322697
C	4.164014	0.081391	0.169215
C	-0.715460	0.970670	-0.570853
C	0.546569	0.982357	0.350831
H	0.200939	0.811177	1.368736
C	1.264449	2.364727	0.297805
H	-2.608550	-3.124986	0.855125
H	-4.823742	-2.059977	1.018508
H	-5.145679	0.271280	0.282512
H	3.052534	-2.965221	-0.783349
H	5.163583	-1.745133	-0.375617
H	5.073398	0.622481	0.352656
C	-1.505231	2.320145	-0.501264
H	-0.387174	0.797351	-1.594710
C	-2.999042	1.973496	-0.675324
H	-1.372965	2.756596	0.481221
H	-1.157828	3.039670	-1.230166
H	-3.296342	2.023840	-1.719589
H	-3.641907	2.650542	-0.125479
C	2.704255	2.116022	0.758675
H	1.274154	2.718016	-0.728613
H	0.765107	3.110376	0.899016
H	3.407738	2.818698	0.328575
H	2.784362	2.199749	1.840045