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

Electronic Supplementary Information

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Appendix 1: Cartesian coordinates for the energy minima of DAS and DAE.

Table S1. Cartesian coordinates of conformer I of DAS obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
S	-0.000018	1.534467	0.000003
C	1.130406	0.354031	0.840024
H	0.540902	-0.321317	1.458241
H	1.728935	0.986679	1.495733
C	-1.130415	0.354016	-0.840026
H	-1.728952	0.986653	-1.495736
H	-0.540898	-0.321321	-1.458244
C	1.984608	-0.389913	-0.128009
H	2.665132	0.213876	-0.718336
C	1.927950	-1.702258	-0.321241
H	2.561567	-2.195851	-1.045172
H	1.250613	-2.326643	0.247540
C	-1.984606	-0.389951	0.128000
H	-2.665159	0.213818	0.718313
C	-1.927902	-1.702292	0.321244
H	-1.250536	-2.326657	-0.247523
H	-2.561512	-2.195902	1.045170

Table S2. Cartesian coordinates of conformer I of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	0.951237	0.658573	-0.728515
C	1.908250	-0.067827	0.167553
C	2.104291	-1.379080	0.141217
H	2.818512	-1.863011	0.793678
H	1.557450	-2.014763	-0.544968
H	2.454832	0.551571	0.871543
O	0.000001	1.433724	0.000001
C	-0.951236	0.658573	0.728515
C	-1.908249	-0.067826	-0.167554
C	-2.104293	-1.379078	-0.141217
H	-2.818515	-1.863008	-0.793679
H	-1.557455	-2.014762	0.544969
H	-2.454829	0.551573	-0.871545
H	-1.485574	1.384296	1.343287
H	-0.448682	-0.048688	1.395505
H	0.448682	-0.048687	-1.395505
H	1.485575	1.384296	-1.343286

Table S3. Cartesian coordinates of conformer II of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.174844	-0.965856	0.000008
C	-2.392997	-0.102340	0.000003
C	-2.396585	1.222526	-0.000007
H	-3.324380	1.777173	-0.000009
H	-1.474457	1.785213	-0.000012
H	-3.329093	-0.651009	0.000008
O	0.000000	-0.188737	-0.000004
C	1.174844	-0.965856	-0.000004
C	2.392997	-0.102340	-0.000005
C	2.396585	1.222526	0.000009
H	3.324380	1.777173	0.000007
H	1.474457	1.785213	0.000020
H	3.329093	-0.651009	-0.000018
H	1.193118	-1.625632	-0.881078
H	1.193120	-1.625630	0.881071
H	-1.193122	-1.625640	-0.881060
H	-1.193116	-1.625622	0.881089

Table S4. Cartesian coordinates of conformer III of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-0.737051	-0.602201	0.387824
C	-2.190651	-0.715259	0.067135
C	-2.949890	0.252462	-0.425890
H	-3.997796	0.086870	-0.633597
H	-2.543823	1.231815	-0.633823
H	-2.616404	-1.692760	0.269330
O	-0.257777	0.696793	0.107506
C	1.117697	0.876225	0.418043
C	2.028572	0.135008	-0.514231
C	2.964731	-0.719291	-0.124866
H	3.614331	-1.215591	-0.832975
H	3.119730	-0.946060	0.923389
H	1.882499	0.341643	-1.569640
H	1.317149	0.581950	1.456070
H	1.287734	1.950822	0.333179
H	-0.176374	-1.354135	-0.183144
H	-0.575096	-0.838514	1.450965

Table S5. Cartesian coordinates of conformer IV of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.228332	-0.913448	-0.057890
C	-2.527804	-0.178843	-0.102289
C	-2.669417	1.136665	-0.032140
H	-3.648069	1.594105	-0.071784
H	-1.812455	1.787420	0.065257
H	-3.399139	-0.817845	-0.201740
O	-0.144569	-0.023112	0.078636
C	1.109858	-0.684031	0.129914
C	2.181863	0.326119	0.370094
C	3.269458	0.449761	-0.376849
H	4.035385	1.177656	-0.147359
H	3.433987	-0.177248	-1.244739
H	2.029124	0.971768	1.228019
H	1.295540	-1.229206	-0.803913
H	1.098441	-1.420484	0.947088
H	-1.114783	-1.512580	-0.974572
H	-1.238483	-1.628751	0.779195

Table S6. Cartesian coordinates of conformer V of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	0.801939	0.047352	-0.457011
C	2.254698	-0.139749	-0.172173
C	3.056900	0.821405	0.262938
H	4.111534	0.648997	0.428219
H	2.685600	1.818595	0.466017
H	2.642673	-1.135578	-0.357059
O	0.069118	-0.959411	0.232398
C	-1.319421	-0.961239	-0.074589
C	-2.043206	0.225904	0.486635
C	-2.778280	1.063362	-0.231810
H	-3.298858	1.897068	0.219526
H	-2.891707	0.937456	-1.302119
H	-1.933880	0.374952	1.556117
H	-1.705261	-1.880640	0.368974
H	-1.470138	-1.016914	-1.160261
H	0.613869	-0.050946	-1.536551
H	0.475100	1.047610	-0.156407

Table S7. Cartesian coordinates of conformer VI of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	0.792343	0.290562	0.164004
C	2.152749	0.187656	-0.439228
C	3.281255	0.398572	0.223134
H	4.244422	0.343725	-0.265245
H	3.280720	0.638327	1.279545
H	2.176156	-0.063966	-1.494002
O	0.080989	-0.912785	-0.105572
C	-1.259606	-0.897063	0.370628
C	-2.147743	0.021561	-0.413582
C	-2.874768	0.995457	0.116704
H	-3.518008	1.621128	-0.487076
H	-2.857284	1.195458	1.181583
H	-2.172204	-0.156285	-1.484021
H	-1.284966	-0.631134	1.434820
H	-1.604876	-1.927540	0.272097
H	0.254508	1.144198	-0.266908
H	0.860235	0.454574	1.246818

Table S8. Cartesian coordinates of conformer VII of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-0.772147	-0.520924	0.738068
C	-2.095122	0.134322	0.519154
C	-2.529472	0.623558	-0.633392
H	-3.502397	1.088475	-0.709788
H	-1.925614	0.568419	-1.527623
H	-2.716065	0.195318	1.406957
O	-0.046851	-0.613529	-0.472874
C	1.298804	-1.005525	-0.299905
C	2.225409	0.116990	0.072506
C	1.895601	1.400108	0.103680
H	2.618137	2.158469	0.370294
H	0.894501	1.727901	-0.142128
H	3.238261	-0.190381	0.314988
H	1.617422	-1.438412	-1.252058
H	1.371809	-1.807907	0.447272
H	-0.922421	-1.526788	1.157741
H	-0.204798	0.049454	1.484476

Table S9. Cartesian coordinates of conformer VIII of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-0.812635	0.134681	-1.010866
C	-1.936238	-0.637249	-0.380905
C	-2.459342	-0.401332	0.813644
H	-3.277060	-0.995976	1.195862
H	-2.088938	0.399014	1.439551
H	-2.331917	-1.440902	-0.995091
O	-0.206267	1.084787	-0.153590
C	0.780484	0.535666	0.721533
C	2.046199	0.187452	-0.000261
C	2.606567	-1.014542	0.014165
H	3.530548	-1.220103	-0.509229
H	2.161113	-1.836182	0.562489
H	2.501766	0.995753	-0.563081
H	0.389826	-0.339338	1.249095
H	0.967872	1.319133	1.457538
H	-1.195012	0.697299	-1.866783
H	-0.064046	-0.562538	-1.405834

Table S10. Cartesian coordinates of conformer IX of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.181606	-0.622797	0.085936
C	-2.366734	0.155731	-0.378854
C	-3.400783	0.468289	0.388832
H	-4.252327	1.009779	0.000482
H	-3.433200	0.189763	1.435177
H	-2.347188	0.455276	-1.421041
O	-0.000001	0.092767	-0.241189
C	1.181605	-0.622792	0.085945
C	2.366733	0.155731	-0.378852
C	3.400786	0.468287	0.388828
H	4.252331	1.009773	0.000472
H	3.433207	0.189763	1.435173
H	2.347182	0.455274	-1.421040
H	1.158450	-1.604882	-0.409973
H	1.237263	-0.800646	1.167233
H	-1.158450	-1.604880	-0.409991
H	-1.237265	-0.800662	1.167223

Table S11. Cartesian coordinates of conformer X of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-0.795993	-0.445946	-0.519555
C	-2.117996	-0.231810	0.137801
C	-2.867955	0.847030	-0.036338
H	-3.834290	0.949117	0.438030
H	-2.542083	1.666338	-0.665684
H	-2.455303	-1.036521	0.782013
O	0.156759	-0.798725	0.479582
C	1.461078	-0.993266	-0.026816
C	2.249974	0.271566	-0.215969
C	1.874027	1.475220	0.191190
H	2.500179	2.341981	0.033156
H	0.931952	1.624811	0.701107
H	3.204652	0.141258	-0.716871
H	1.423170	-1.548460	-0.974599
H	1.977177	-1.636968	0.690975
H	-0.485224	0.453665	-1.058515
H	-0.864074	-1.266427	-1.248451

Table S12. Cartesian coordinates of conformer XI of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-0.701775	-0.958524	-0.017614
C	-2.070034	-0.514090	0.411541
C	-2.663859	0.611736	0.043025
H	-3.657306	0.861367	0.387923
H	-2.174666	1.311512	-0.620567
H	-2.583783	-1.207068	1.071358
O	0.000000	-0.000003	-0.789168
C	0.701773	0.958522	-0.017615
C	2.070034	0.514093	0.411539
C	2.663861	-0.611733	0.043027
H	3.657310	-0.861361	0.387924
H	2.174669	-1.311513	-0.620563
H	2.583783	1.207074	1.071352
H	0.114863	1.249375	0.861640
H	0.789394	1.852959	-0.640726
H	-0.789400	-1.852961	-0.640725
H	-0.114865	-1.249379	0.861641

Table S13. Cartesian coordinates of conformer XII of DAE obtained at the B3LYP-D3(BJ)/aug-cc pVTZ level.

	Cartesian Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.339497	-1.067501	0.051339
C	-2.338214	0.015119	-0.245697
C	-2.195774	1.295658	0.063710
H	-2.964114	2.019003	-0.169912
H	-1.308220	1.655109	0.566321
H	-3.242440	-0.324941	-0.741727
O	-0.098502	-0.603430	0.542677
C	0.793985	-0.174889	-0.482938
C	1.964949	0.500045	0.148116
C	3.228198	0.169192	-0.078222
H	4.046645	0.708189	0.378724
H	3.488414	-0.652874	-0.733923
H	1.725988	1.317964	0.819266
H	0.278492	0.523030	-1.153250
H	1.119425	-1.035581	-1.079380
H	-1.189535	-1.684570	-0.845340
H	-1.744515	-1.731214	0.820202

Appendix 2: Dihedral angle values for the conformers of DAS and DAE.

Table S14. Dihedral angle values (in degrees) for the 24 conformers of DAS obtained at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

DAS	ø	δ	θ	γ
I	-115.5	68.7	68.7	-115.5
II	-9.2	-71.5	-63.2	111.2
III	115.4	73.6	63.2	-112.4
IV	112.7	161.0	-67.3	130.0
V	-114.3	64.9	166.8	112.7
VI	115.8	99.5	-62.7	115.9
VII	-122.8	58.7	-94.6	122.5
VIII	2.6	-174.0	67.7	-114.0
IX	3.2	97.9	-58.0	117.2
X	8.9	72.9	-161.9	-112.1
XI	-113.2	-165.2	-71.8	-8.9
XII	-112.4	-166.9	166.9	112.4
XIII	-112.2	-166.2	-166.2	-112.2
XIV	-114.6	-71.1	-162.2	-112.4
XV	9.7	72.8	72.8	9.7
XVI	10.1	70.9	75.8	116.2
XVII	112.1	166.8	-78.0	-116.7
XVII	-111.9	-63.7	-63.7	-111.9
XIX	3.1	88.6	-76.0	-113.2
XX	117.5	98.3	-68.9	-111.7
XXI	8.3	73.5	-172.6	4.2
XXII	-0.2	179.1	167.1	112.8
XXIII	-0.7	176.2	75.1	115.8
XXIV	0.0	-180.0	180.0	0.0

Table S15. Dihedral angle values (in degrees) for the 23 conformers of DAE obtained at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

DAE	ø	δ	θ	γ
I	124.3	-69.1	-69.1	124.3
II	0.0	-180.0	-180.0	0.0
III	0.6	178.8	70.5	-125.9
IV	0.4	179.8	-176.1	-127.7
V	-128.3	-174.0	-70.2	125.1
VI	-127.3	-177.1	70.8	-125.2
VII	-2.7	169.5	-82.4	-7.3
VIII	-124.6	73.5	82.7	7.2
IX	-127.9	-176	176.0	127.9
X	8.1	82.3	-178.5	128.9
XI	5.4	85.2	85.2	5.4
XII	-8.5	-82.5	170.6	126.3
XIII	2.0	110.3	-65.1	124.1
XIV	125.1	-70.1	-81.0	-121.8
XV	-0.1	-174.6	-77.8	-120.4
XVI	-131.1	94.1	-67.0	131.8
XVII	-124.7	70.8	-99.1	-119.2
XVII	119.5	75.6	169.4	127.7
XIX	-120.2	-78.8	179.8	127.3
XX	123.9	88.2	82.9	6.0
XXI	-0.4	-103.9	74.2	120.9
XXII	-123.2	-85.5	-85.5	-123.2
XXIII	-112.9	-61.5	-61.5	-112.9

Appendix 3: Calculated energetic and spectroscopic parameters for the conformer I of DAS and conformers I–IX of DAE.

Table S16. Calculated rotational and quartic centrifugal distortion constants for the observed conformer I of DAS at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

Parameter	Conformer I
A/MHz	2449
B/MHz	1781
C/MHz	1186
Δ_J/kHz	2.3091
Δ_{JK}/kHz	-6.4743
Δ_K/kHz	4.4152
δ_J/kHz	-0.1330
δ_K/kHz	-3.6296
$\mu_a/\mu_b/\mu_c$	0.0/1.2/0.0

Table S17. Calculated rotational and quartic centrifugal distortion constants for the observed nine conformers of DAE at the B3LYP-D3(BJ)/aug-cc-pVTZ level of theory.

Parameter	Conformer I	Conformer II	Conformer III	Conformer IV	Conformer V
A/MHz	3784	5842	7505	8059	6276
B/MHz	1817	1379	1208	1104	1198
C/MHz	1396	1131	1129	1010	1078
Δ_J/kHz	3.5690	0.2520	0.4395	0.1694	0.5049
Δ_{JK}/kHz	-16.4878	-1.4424	-12.9036	-4.8265	-9.7321
Δ_K/kHz	26.5201	8.0525	162.9582	79.1911	85.3018
δ_J/kHz	1.2760	0.0647	-0.0037	0.0203	0.1151
δ_K/kHz	3.0050	0.7390	4.9686	-0.8750	1.3339
$\mu_a/\mu_b/\mu_c$	0.0/1.2/0.0	0.0/1.6/0.0	1.1/0.9/0.5	0.3/1.3/0.0	0.6/0.7/0.7

Parameter	Conformer VI	Conformer VII	Conformer VIII	Conformer IX
A/MHz[a]	7493	5214	5204	11535
B/MHz	1125	1501	1422	932
C/MHz	1055	1352	1380	924
Δ_J/kHz[b]	0.2566	2.1594	1.2606	0.1331
Δ_{JK}/kHz	-4.6709	-17.3745	-14.5056	-13.8276
Δ_K/kHz	71.5381	68.0071	60.7118	535.8620
δ_J/kHz	0.0502	0.6488	0.1839	-0.0103
δ_K/kHz	0.3554	6.7428	-5.0927	-6.4307
$\mu_a/\mu_b/\mu_c$[c]	0.7/0.9/0.4	0.7/0.6/1.1	0.5/1.1/0.2	0.0/1.1/0.4

Appendix 4: Assigned transitions for the observed species of conformer I of DAS and conformers I–IX of DAE.

Table S18. Assigned transitions for the parent species of conformer I of DAS

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
6	4	3	6	3	4	7180.7599	0.0004
6	5	1	6	4	2	7487.7198	-0.0001
3	1	2	2	2	1	7580.3748	0.0006
3	1	2	2	2	1	7580.3751	0.0009
3	0	3	2	1	2	7732.4123	-0.0005
5	2	4	5	1	5	7774.4837	-0.0038
6	3	4	6	2	5	7787.5076	0.0001
5	5	0	5	4	1	8006.9357	-0.0004
8	3	5	8	2	6	8023.9536	0.0009
7	4	4	7	3	5	8062.1770	0.0009
6	5	2	6	4	3	8136.4923	0.0005
5	5	1	5	4	2	8169.0923	0.0002
3	1	3	2	0	2	8173.6139	-0.0003
7	5	3	7	4	4	8280.9563	0.0001
2	2	1	1	1	0	8524.2260	-0.0008
8	5	4	8	4	5	8729.5906	0.0001
7	2	5	7	1	6	8904.0984	-0.0003
8	6	2	8	5	3	8935.8383	0.0020
7	3	5	7	2	6	9318.8845	0.0003
6	1	5	6	0	6	9375.2302	-0.0009
2	2	0	1	1	1	9390.5713	-0.0017
6	2	5	6	1	6	9460.1206	-0.0018
9	5	5	9	4	6	9555.8810	0.0004
7	6	1	7	5	2	9587.5855	0.0002

8	6	3	8	5	4	9738.7936	0.0001
7	6	2	7	5	3	9825.4581	0.0004
9	6	4	9	5	5	9827.9912	-0.0002
6	6	0	6	5	1	9919.1566	0.0015
6	6	1	6	5	2	9965.2995	0.0000
4	0	4	3	1	3	10250.0357	-0.0007
4	1	4	3	0	3	10398.7378	-0.0005
10	5	6	10	4	7	10750.6028	0.0001
9	4	6	9	3	7	10801.3136	0.0013
8	2	6	8	1	7	10840.7954	0.0010
3	2	2	2	1	1	10885.7754	0.0000
4	1	3	3	2	2	10970.3425	0.0000
8	3	6	8	2	7	10990.7879	0.0000
7	1	6	7	0	7	11167.9325	-0.0001
6	3	4	5	4	1	11174.9884	-0.0007
7	2	6	7	1	7	11192.9150	-0.0002
10	7	4	10	6	5	11291.4692	-0.0015
9	7	3	9	6	4	11430.2396	-0.0012
8	7	1	8	6	2	11549.7472	-0.0006
8	7	2	8	6	3	11622.8550	-0.0003
10	3	7	10	2	8	12239.5408	-0.0036
10	4	7	10	3	8	12466.6631	0.0002
5	0	5	4	1	4	12663.1419	-0.0005
9	2	7	9	1	8	12677.3052	0.0012
5	1	5	4	0	4	12705.3031	-0.0005
9	3	7	9	2	8	12725.3785	0.0008
8	1	7	8	0	8	12934.0691	0.0005
8	2	7	8	1	8	12940.8770	0.0001
4	2	3	3	1	2	12952.4847	0.0006
10	8	2	10	7	3	13138.0291	0.0030
5	2	3	4	3	2	13235.1006	0.0017

10	8	3	10	7	4	13237.5660	-0.0028
7	4	4	6	5	1	13366.4441	0.0000
3	3	1	2	2	0	13597.8489	0.0006
5	1	4	4	2	3	13978.6016	0.0000
10	2	8	10	1	9	14466.8814	0.0002
10	3	8	10	2	9	14481.0933	0.0004
6	3	3	5	4	2	14571.5099	0.0004
9	1	8	9	0	9	14690.4665	0.0011
9	2	8	9	1	9	14692.2215	-0.0016
5	2	4	4	1	3	14913.9293	-0.0001
6	0	6	5	1	5	15039.0650	-0.0001
6	1	6	5	0	5	15049.8980	-0.0002
4	3	2	3	2	1	16095.7896	0.0001
10	1	9	10	0	0	16443.0824	0.0002
10	2	9	10	1	0	16443.5183	0.0002
6	1	5	5	2	4	16639.8090	0.0001
6	2	4	5	3	3	16974.2978	0.0003
6	2	5	5	1	4	16991.7400	-0.0001
7	0	7	6	1	6	17403.9734	0.0000
7	1	7	6	0	6	17406.5913	0.0000
9	4	6	8	5	3	17508.6877	-0.0009
4	3	1	3	2	2	17685.2828	0.0000
3	3	1	2	0	2	17988.7663	-0.0004
4	4	1	3	3	0	18609.9738	0.0004
4	4	0	3	3	1	18711.3040	0.0005
7	3	4	6	4	3	18936.0021	-0.0002
7	1	6	6	2	5	19111.7837	0.0000
7	2	6	6	1	5	19224.2754	0.0001
8	0	8	7	1	7	19765.9991	0.0007
8	1	8	7	0	7	19766.6058	0.0006
6	3	4	5	2	3	19970.2301	-0.0007

7	2	5	6	3	4	20228.3754	0.0004

Table S19. Assigned transitions for the ^{13}C1 isotopic species of conformer I of DAS

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
6	4	3	6	3	4	7150.7321	-0.0014
3	0	3	2	1	2	7697.7302	-0.0004
6	3	4	6	2	5	7722.2295	0.0019
3	1	3	2	0	2	8146.3871	-0.0004
7	5	3	7	4	4	8265.8509	0.0002
2	2	1	1	1	0	8492.1918	-0.0019
2	2	0	1	1	1	9343.9021	0.0030
6	2	5	6	1	6	9371.4927	-0.0022
4	0	4	3	1	3	10209.8881	-0.0007
4	1	4	3	0	3	10362.9166	-0.0002
3	2	2	2	1	1	10846.2263	-0.0001
4	1	3	3	2	2	10898.1361	0.0011
5	0	5	4	1	4	12616.7969	-0.0004
5	1	5	4	0	4	12660.7182	-0.0010
4	2	3	3	1	2	12908.7294	0.0014
5	2	3	4	3	2	13118.8710	-0.0010
3	3	1	2	2	0	13545.9798	-0.0007
3	3	0	2	2	1	13881.4144	0.0005
5	1	4	4	2	3	13904.1393	0.0001
5	2	4	4	1	3	14863.4460	-0.0013
6	0	6	5	1	5	14985.7727	-0.0003
6	1	6	5	0	5	14997.1974	0.0008
4	3	2	3	2	1	16037.4853	0.0006
6	1	5	5	2	4	16564.3330	0.0011
6	2	5	5	1	4	16929.9448	0.0005
7	0	7	6	1	6	17343.3629	-0.0007

7	1	7	6	0	6	17346.1577	-0.0001
4	3	1	3	2	2	17587.0650	0.0007
5	3	3	4	2	2	18117.6398	-0.0011
4	4	1	3	3	0	18536.9384	0.0007
4	4	0	3	3	1	18634.2678	-0.0009
7	1	6	6	2	5	19032.7479	0.0001
7	2	6	6	1	5	19151.1214	0.0019
8	0	8	7	1	7	19697.9332	-0.0005
8	1	8	7	0	7	19698.5888	-0.0003

Table S20. Assigned transitions for the ^{13}C2 isotopic species of conformer I of DAS

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
6	4	3	6	3	4	7240.3477	-0.0009
3	0	3	2	1	2	7641.5826	-0.0002
6	3	4	6	2	5	7747.7068	0.0013
3	1	3	2	0	2	8116.3106	-0.0004
6	5	2	6	4	3	8296.1335	-0.0005
7	5	3	7	4	4	8411.4287	-0.0001
2	2	1	1	1	0	8507.7219	-0.0006
2	2	0	1	1	1	9346.4026	-0.0008
6	2	5	6	1	6	9381.0340	-0.0010
7	6	1	7	5	2	9835.7505	0.0003
7	6	2	7	5	3	10038.4191	-0.0001
4	0	4	3	1	3	10147.1380	-0.0001
4	1	4	3	0	3	10313.1982	0.0000
3	2	2	2	1	1	10847.3208	0.0017
5	0	5	4	1	4	12543.6807	-0.0003
5	1	5	4	0	4	12592.5966	-0.0006
4	2	3	3	1	2	12896.3680	0.0015

3	3	1	2	2	0	13578.2367	-0.0010
5	1	4	4	2	3	13796.8786	0.0011
3	3	0	2	2	1	13901.1169	0.0000
5	2	4	4	1	3	14830.2335	-0.0028
6	0	6	5	1	5	14899.8331	-0.0007
6	1	6	5	0	5	14912.8891	-0.0001
4	3	2	3	2	1	16060.5139	0.0007
6	1	5	5	2	4	16463.4572	0.0009
6	2	4	5	3	3	16651.4492	-0.0007
6	2	5	5	1	4	16868.1453	0.0010
7	0	7	6	1	6	17243.5221	0.0004
7	1	7	6	0	6	17246.7980	-0.0003
4	3	1	3	2	2	17558.8233	0.0004
5	3	3	4	2	2	18133.2218	0.0000
4	4	1	3	3	0	18581.8073	0.0004
4	4	0	3	3	1	18672.9772	0.0004
7	1	6	6	2	5	18928.8269	-0.0001
7	2	6	6	1	5	19063.4723	0.0003
8	0	8	7	1	7	19583.8063	-0.0004
8	1	8	7	0	7	19584.5959	0.0005

Table S21. Assigned transitions for the ^{13}C3 isotopic species of conformer I of DAS

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
6	4	3	6	3	4	7093.2021	0.0006
3	0	3	2	1	2	7617.2028	0.0002
3	1	3	2	0	2	8051.5592	0.0004
7	5	3	7	4	4	8176.8862	0.0000
2	2	1	1	1	0	8405.5084	-0.0003
8	5	4	8	4	5	8622.9062	-0.0003

6	2	5	6	1	6	9352.5035	0.0004
7	6	2	7	5	3	9698.9507	-0.0003
4	0	4	3	1	3	10096.2305	0.0000
4	1	4	3	0	3	10242.3455	0.0002
3	2	2	2	1	1	10730.7895	-0.0017
4	1	3	3	2	2	10812.3388	0.0000
7	1	6	7	0	7	11041.2572	-0.0004
7	2	6	7	1	7	11065.6791	-0.0007
5	0	5	4	1	4	12472.2024	-0.0001
5	1	5	4	0	4	12513.5489	0.0000
4	2	3	3	1	2	12764.5017	-0.0028
5	2	3	4	3	2	13047.8662	-0.0005
3	3	1	2	2	0	13409.9392	0.0003
3	3	0	2	2	1	13751.8208	0.0008
5	1	4	4	2	3	13775.1725	-0.0001
5	2	4	4	1	3	14694.7176	0.0008
6	0	6	5	1	5	14811.5878	-0.0001
6	1	6	5	0	5	14822.1916	0.0008
4	3	2	3	2	1	15869.6855	-0.0005
6	1	5	5	2	4	16395.2388	-0.0001
6	2	4	5	3	3	16732.9905	0.0001
6	2	5	5	1	4	16740.5194	0.0005
7	0	7	6	1	6	17140.1581	-0.0004
7	1	7	6	0	6	17142.7150	-0.0008
4	3	1	3	2	2	17445.1058	0.0007
5	3	3	4	2	2	17917.8245	-0.0002
4	4	1	3	3	0	18353.8803	0.0002
4	4	0	3	3	1	18454.5516	0.0008
7	1	6	6	2	5	18828.9138	0.0006
7	2	6	6	1	5	18939.0531	0.0016
8	0	8	7	1	7	19465.9038	-0.0009

Table S22. Assigned transitions for the ^{34}S Isotopic species of conformer I of DAS

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
6	4	3	6	3	4	6944.3377	-0.0010
3	0	3	2	1	2	7687.2445	0.0006
6	5	2	6	4	3	7693.1414	0.0001
6	3	4	6	2	5	7714.7828	-0.0017
5	2	4	5	1	5	7728.9854	-0.0012
7	4	4	7	3	5	7908.7695	0.0004
3	1	3	2	0	2	8062.6173	-0.0006
2	2	1	1	1	0	8351.5247	-0.0012
2	2	0	1	1	1	9253.1370	0.0010
4	0	4	3	1	3	10159.2329	-0.0004
4	1	4	3	0	3	10276.9775	-0.0006
4	1	3	3	2	2	11017.6451	0.0002
5	0	5	4	1	4	12537.2583	-0.0004
5	1	5	4	0	4	12568.2771	-0.0005
4	2	3	3	1	2	12728.2315	0.0000
3	3	1	2	2	0	13313.1352	-0.0003
5	2	3	4	3	2	13472.3673	-0.0006
3	3	0	2	2	1	13694.5405	0.0000
5	1	4	4	2	3	13931.1191	-0.0001
5	2	4	4	1	3	14685.6890	-0.0002
6	0	6	5	1	5	14884.3472	-0.0008
6	1	6	5	0	5	14891.7560	-0.0001
4	3	2	3	2	1	15771.5338	0.0008
6	1	5	5	2	4	16514.4390	-0.0002
6	2	5	5	1	4	16777.2748	0.0002
6	2	4	5	3	3	17094.8694	0.0010
7	0	7	6	1	6	17222.9705	-0.0002

7	1	7	6	0	6	17224.6347	-0.0004
4	3	1	3	2	2	17506.3914	0.0030
5	3	3	4	2	2	17810.9086	-0.0008
4	4	1	3	3	0	18225.0297	0.0000
4	4	0	3	3	1	18345.6921	-0.0004
7	1	6	6	2	5	18934.6120	-0.0002
7	2	6	6	1	5	19012.4231	-0.0007
8	0	8	7	1	7	19559.5518	0.0003
8	1	8	7	0	7	19559.9104	0.0003
6	3	4	5	2	3	19578.8642	0.0019

Table S23. Assigned transitions for the parent species of conformer I of DAE

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
2	2	1	2	1	2	7170.7661	-0.0012
3	0	3	2	1	2	7780.8672	-0.0005
3	2	2	3	1	3	7839.6831	-0.0021
2	1	2	1	0	1	7962.1138	-0.0004
8	3	5	8	2	6	8202.4262	0.0029
9	3	6	9	2	7	8320.2886	0.0032
8	2	6	8	1	7	8504.9001	-0.0004
7	3	4	7	2	5	8510.7975	0.0000
6	1	5	6	0	6	8681.6909	0.0018
4	2	3	4	1	4	8743.1272	-0.0034
6	3	3	6	2	4	9085.1816	0.0004
5	3	2	5	2	3	9733.5625	-0.0013
5	2	4	5	1	5	9878.1483	-0.0017
4	3	1	4	2	2	10283.8320	-0.0004
3	1	3	2	0	2	10562.1785	0.0000
3	3	0	3	2	1	10640.3874	-0.0005

3	3	1	3	2	2	10931.1756	-0.0001
4	3	2	4	2	3	11086.2120	0.0007
4	0	4	3	1	3	11111.9207	0.0002
6	2	5	6	1	6	11230.1885	-0.0001
5	3	3	5	2	4	11379.2913	0.0010
6	3	4	6	2	5	11852.5169	0.0019
5	1	4	4	2	3	12204.4488	0.0007
7	3	5	7	2	6	12538.1393	0.0031
2	2	1	1	1	0	12742.5681	-0.0003
7	2	6	7	1	7	12772.7830	0.0014
4	1	4	3	0	3	13054.6373	-0.0006
2	2	0	1	1	1	13225.4982	-0.0015
5	0	5	4	1	4	14311.2948	0.0008
7	4	3	7	3	4	14261.2697	0.0001
6	4	2	6	3	3	14725.5089	0.0002
5	4	1	5	3	2	14990.0866	0.0006
4	4	0	4	3	1	15119.4376	0.0003
5	4	2	5	3	3	15136.1964	0.0028
6	4	3	6	3	4	15137.1323	0.0005
4	4	1	4	3	2	15157.4203	0.0000
7	2	5	6	3	4	15170.3909	-0.0021
7	4	4	7	3	5	15195.3849	-0.0033
8	4	5	8	3	6	15355.3896	-0.0015
3	2	2	2	1	1	15528.5792	-0.0015
5	1	5	4	0	4	15537.3831	-0.0003
9	4	6	9	3	7	15664.1560	-0.0036
6	1	5	5	2	4	16174.1043	0.0009
6	0	6	5	1	5	17370.5656	0.0012
6	1	6	5	0	5	18081.3980	0.0006
4	2	3	3	1	2	18097.1392	0.0012

Table S24. Assigned transitions for the ^{13}C1 isotopic species of conformer I of DAE

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
3	0	3	2	1	2	7755.6882	-0.0001
3	2	2	3	1	3	7768.1859	-0.0034
2	1	2	1	0	1	7920.6355	0.0026
3	1	3	2	0	2	10512.5656	-0.0015
4	3	2	4	2	3	10985.9294	0.0017
4	0	4	3	1	3	11071.8445	-0.0038
5	3	3	5	2	4	11276.0705	-0.0018
2	2	1	1	1	0	12657.6988	-0.0020
4	1	4	3	0	3	12997.8724	-0.0021
2	2	0	1	1	1	13135.9814	-0.0007
5	0	5	4	1	4	14257.6466	0.0015
5	1	5	4	0	4	15473.4886	0.0003
3	2	1	2	1	2	16981.1913	0.0029
6	0	6	5	1	5	17304.6686	0.0016
4	2	3	3	1	2	17994.5670	0.0036
6	1	6	5	0	5	18009.7398	-0.0021

Table S25. Assigned transitions for the ^{13}C2 isotopic species of conformer I of DAE.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
3	2	2	3	1	3	7861.4599	-0.0032
4	3	1	4	2	2	10399.0437	-0.0019
3	1	3	2	0	2	10496.4700	0.0003
4	0	4	3	1	3	10956.8065	-0.0037
4	3	2	4	2	3	11164.0705	0.0006
5	3	3	5	2	4	11443.1931	0.0011
2	2	1	1	1	0	12726.0336	0.0022

4	1	4	3	0	3	12964.5917	-0.0016
2	2	0	1	1	1	13196.1702	-0.0021
5	0	5	4	1	4	14134.7852	0.0014
5	1	5	4	0	4	15418.9943	-0.0001
3	2	2	2	1	1	15484.7783	0.0040
6	0	6	5	1	5	17175.1867	0.0022
6	1	6	5	0	5	17930.6467	-0.0019

Table S26. Assigned transitions for the $^{13}C3$ isotopic species of conformer I of DAE.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
3	2	2	3	1	3	7747.3297	0.0013
2	1	2	1	0	1	7838.6276	0.0010
3	1	3	2	0	2	10393.2059	-0.0001
4	0	4	3	1	3	10922.3095	-0.0008
4	3	2	4	2	3	10955.0753	0.0019
5	3	3	5	2	4	11244.8696	-0.0019
2	2	1	1	1	0	12562.6223	-0.0024
4	1	4	3	0	3	12841.4555	0.0031
2	2	0	1	1	1	13040.0303	-0.0023
5	0	5	4	1	4	14069.1267	0.0000
5	1	5	4	0	4	15280.1440	-0.0031
3	2	1	2	1	2	16845.6255	0.0007
6	0	6	5	1	5	17077.4609	0.0013
6	1	6	5	0	5	17779.4366	-0.0007
4	2	3	3	1	2	17824.4309	0.0021

Table S27. Assigned transitions for the parent species of conformer II of DAE.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
1	1	1	0	0	0	6917.6622	-0.0019
7	1	6	6	2	5	7470.8108	-0.0014
5	0	5	4	1	4	9069.8674	0.0008
2	1	2	1	0	1	9196.2088	-0.0007
8	1	7	8	0	8	10512.8007	0.0010
8	1	7	7	2	6	10847.2913	-0.0002
3	1	3	2	0	2	11352.4680	-0.0005
9	2	7	9	1	8	11359.1432	-0.0014
7	2	5	7	1	6	11423.5961	0.0012
6	2	4	6	1	5	11692.6246	0.0003
6	0	6	5	1	5	11924.2246	0.0004
5	2	3	5	1	4	12053.5069	0.0006
9	1	8	9	0	9	12300.7832	0.0023
4	2	2	4	1	3	12452.7865	0.0014
4	1	4	3	0	3	13400.1281	0.0000
2	2	1	2	1	2	13917.2795	-0.0010
9	1	8	8	2	7	14273.5016	0.0010
7	0	7	6	1	6	14749.7539	0.0003
4	2	3	4	1	4	14820.7539	0.0029
5	1	5	4	0	4	15360.9012	0.0000
5	2	4	5	1	5	15472.7621	0.0024
6	2	5	6	1	6	16260.8371	0.0000
7	2	6	7	1	7	17185.9283	-0.0008
6	1	6	5	0	5	17263.2758	0.0010
8	0	8	7	1	7	17520.4215	0.0005
10	1	9	9	2	8	17724.1511	-0.0014
8	2	7	8	1	8	18247.6218	-0.0036
2	2	1	1	1	0	18474.3681	-0.0021

2	2	0	1	1	1	18737.7753	-0.0019
7	1	7	6	0	6	19139.6121	0.0015

Table S28. Assigned transitions for the parent species of conformer III of DAE.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
1	1	0	1	0	1	6341.1443	0.0018
2	1	1	2	0	2	6422.6714	-0.0012
3	1	2	3	0	3	6546.4171	-0.0012
4	1	3	4	0	4	6714.1098	-0.0009
3	1	3	2	1	2	6920.4585	0.0002
3	0	3	2	0	2	7038.8404	-0.0002
3	2	1	2	2	0	7045.3059	0.0030
6	0	6	5	1	4	7128.5293	-0.0039
3	1	2	2	1	1	7162.5858	-0.0006
6	1	5	6	0	6	7191.0221	0.0036
7	1	6	7	0	7	7506.3569	-0.0028
6	0	6	5	1	5	8339.0598	-0.0012
1	1	1	0	0	0	8607.7559	-0.0015
1	1	0	0	0	0	8688.4682	-0.0007
4	1	4	3	1	3	9226.3409	0.0003
4	0	4	3	0	3	9381.4621	0.0000
4	2	3	3	2	2	9388.9567	-0.0008
4	3	2	3	3	1	9391.5326	0.0023
4	3	1	3	3	0	9391.5617	0.0035
4	2	2	3	2	1	9396.7033	-0.0004
4	1	3	3	1	2	9549.1536	-0.0009
2	1	2	1	0	1	10874.4058	-0.0007
7	0	7	6	1	6	10891.0777	0.0008
2	1	1	1	0	1	11116.5395	-0.0013

8	0	8	7	1	6	11206.9307	-0.0011
5	1	5	4	1	4	11531.4345	0.0005
5	0	5	4	0	4	11720.9584	0.0001
5	2	4	4	2	3	11735.1573	-0.0005
5	4	1	4	4	0	11739.9058	0.0018
5	4	2	4	4	1	11739.9058	0.0019
5	3	3	4	3	2	11740.0385	0.0010
5	3	2	4	3	1	11740.1340	-0.0011
5	2	3	4	2	2	11750.6359	-0.0008
5	1	4	4	1	3	11934.8847	-0.0005
3	1	3	2	0	2	13100.9965	0.0000
8	0	8	7	1	7	13465.8265	0.0023
3	1	2	2	0	2	13585.2565	-0.0024
6	1	6	5	1	5	13835.5586	0.0005
6	0	6	5	0	5	14056.5719	0.0008
6	2	5	5	2	4	14080.6658	-0.0002
6	4	3	5	4	2	14088.3461	-0.0025
6	4	2	5	4	1	14088.3461	-0.0033
6	3	4	5	3	3	14088.9344	-0.0013
6	3	3	5	3	2	14089.1955	-0.0004
6	2	4	5	2	3	14107.7108	-0.0004
6	1	5	5	1	4	14319.5518	0.0000
4	1	4	3	0	3	15288.4978	0.0013
9	0	9	8	1	8	16058.7129	-0.0012
4	1	3	3	0	3	16095.5712	-0.0016
7	1	7	6	1	6	16138.5444	0.0001
7	0	7	6	0	6	16387.5749	0.0009
7	2	6	6	2	5	16425.3432	-0.0004
7	4	3	6	4	2	16437.0485	-0.0004
7	4	4	6	4	3	16437.0485	0.0022
7	3	5	6	3	4	16438.2780	-0.0002

7	3	4	6	3	3	16438.8633	-0.0002
7	2	5	6	2	4	16468.5053	0.0000
7	1	6	6	1	5	16702.9162	0.0010
5	1	5	4	0	4	17438.4685	0.0002
8	1	8	7	1	7	18440.2371	0.0000
5	1	4	4	0	4	18648.9969	0.0009
8	0	8	7	0	7	18713.2933	0.0017
8	2	7	7	2	6	18769.0537	0.0004
8	3	6	7	3	5	18788.1046	-0.0005
8	3	5	7	3	4	18789.2734	-0.0013
8	2	6	7	2	5	18833.5454	0.0002
6	1	6	5	0	5	19553.0705	0.0023

Table S29. Assigned transitions for the parent species of conformer IV of DAE.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
2	1	1	2	0	2	7064.2598	0.0001
3	1	2	3	0	3	7210.2820	0.0022
4	1	3	4	0	4	7408.3827	0.0006
5	1	4	5	0	5	7661.4545	0.0006
6	1	5	6	0	6	7973.0463	0.0000
7	1	6	7	0	7	8347.3126	-0.0007
4	0	4	3	0	3	8492.2806	0.0001
4	2	3	3	2	2	8501.4843	-0.0005
4	2	2	3	2	1	8511.2827	-0.0018
4	1	3	3	1	2	8690.3815	-0.0012
8	1	7	8	0	8	8788.9183	0.0007
7	0	7	6	1	6	8847.8441	0.0025
1	1	1	0	0	0	8998.5394	-0.0030
5	1	5	4	1	4	10385.5982	0.0012

5	0	5	4	0	4	10607.9880	0.0005
5	2	4	4	2	3	10625.5959	-0.0005
5	2	3	4	2	2	10645.1752	-0.0008
5	1	4	4	1	3	10861.0581	-0.0011
2	1	2	1	0	1	11028.9667	-0.0005
8	0	8	7	1	7	11237.0624	0.0001
6	1	6	5	1	5	12460.0747	0.0009
6	0	6	5	0	5	12718.8296	0.0008
3	2	1	4	1	4	12742.5673	0.0000
3	1	3	2	0	2	13012.2035	-0.0006
9	0	9	8	1	8	13645.9345	-0.0017
7	1	7	6	1	6	14533.1665	0.0009
7	0	7	6	0	6	14823.9042	0.0003
4	1	4	3	0	3	14949.4888	0.0004
7	1	6	6	1	5	15198.1705	-0.0003
10	0	10	9	1	9	16068.3305	-0.0014
8	1	8	7	1	7	16604.6891	0.0010
5	1	5	4	0	4	16842.8047	0.0000
8	0	8	7	0	7	16922.3865	0.0002
8	2	7	7	2	6	16992.2265	-0.0004
8	1	7	7	1	6	17363.9909	0.0004
11	0	11	10	1	10	18497.9009	0.0007
9	1	9	8	1	8	18674.4754	-0.0016
6	1	6	5	0	5	18694.8915	0.0004
9	0	9	8	0	8	19013.5623	0.0001
9	1	8	8	1	7	19527.5410	0.0010

Table S30. Assigned transitions for the parent species of conformer V of DAE.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
5	0	5	4	1	4	6956.5395	0.0000
7	1	6	7	0	7	7019.9563	-0.0014
3	1	2	2	1	1	7060.7232	0.0002
1	1	1	0	0	0	7279.9820	-0.0015
1	1	0	0	0	0	7404.9010	-0.0018
6	0	6	5	1	4	7616.9361	-0.0020
8	1	7	8	0	8	7657.9216	0.0015
9	1	8	8	2	6	7676.1581	-0.0001
9	1	8	8	2	7	8152.2016	-0.0004
4	1	4	3	1	3	8912.0019	0.0004
4	0	4	3	0	3	9143.1777	0.0005
4	2	3	3	2	2	9164.7815	0.0000
4	3	2	3	3	1	9171.4955	-0.0016
4	3	1	3	3	0	9171.6559	-0.0023
4	1	3	3	1	2	9411.4632	0.0004
7	0	7	6	1	5	9425.6808	0.0008
2	1	2	1	0	1	9446.6948	0.0001
6	0	6	5	1	5	9489.7842	0.0000
2	1	1	1	0	1	9821.4459	-0.0010
10	1	9	9	2	7	10265.6731	-0.0007
10	1	9	9	2	8	11005.1428	-0.0001
8	0	8	7	1	6	11123.7553	-0.0006
5	1	5	4	1	4	11135.7695	0.0005
5	3	3	6	2	4	11371.2898	0.0025
5	3	2	6	2	4	11372.0386	0.0000
5	0	5	4	0	4	11411.6940	0.0007
5	2	4	4	2	3	11452.9930	0.0004
5	4	1	4	4	0	11464.3723	0.0017

5	3	3	4	3	2	11466.2735	0.0006
5	3	2	4	3	1	11466.8351	-0.0011
5	2	3	4	2	2	11499.0724	0.0003
5	3	3	6	2	5	11532.2312	-0.0013
5	3	2	6	2	5	11532.9865	0.0025
3	1	3	2	0	2	11551.8310	0.0005
5	1	4	4	1	3	11759.6929	0.0003
7	0	7	6	1	6	12046.3502	0.0005
3	1	2	2	0	2	12301.2926	0.0008
12	2	10	12	1	11	12682.9429	0.0002
9	0	9	8	1	7	12701.4267	0.0007
11	2	9	11	1	10	12776.2649	0.0001
10	2	8	10	1	9	12943.7947	-0.0007
8	2	7	8	1	7	12959.6231	0.0000
9	2	7	9	1	8	13169.3346	-0.0006
6	1	6	5	1	5	13356.8603	0.0004
8	2	6	8	1	7	13435.6666	-0.0001
7	2	6	7	1	6	13437.1591	0.0000
4	1	4	3	0	3	13598.3312	0.0002
6	0	6	5	0	5	13669.0142	0.0004
4	3	2	5	2	3	13724.4038	-0.0008
4	3	1	5	2	3	13724.5907	-0.0019
7	2	5	7	1	6	13725.1931	0.0000
6	2	5	5	2	4	13739.2174	0.0002
6	4	3	5	4	2	13758.8041	-0.0005
6	4	2	5	4	1	13758.8114	-0.0025
6	3	4	5	3	3	13762.1714	-0.0002
6	3	3	5	3	2	13763.6725	0.0000
4	3	2	5	2	4	13805.1771	0.0002
4	3	1	5	2	4	13805.3636	-0.0012
6	2	4	5	2	3	13819.3906	0.0003

6	2	5	6	1	5	13859.7338	-0.0004
6	2	4	6	1	5	14020.6797	0.0001
6	1	5	5	1	4	14104.6838	0.0004
5	2	4	5	1	4	14225.2004	0.0000
5	2	3	5	1	4	14305.9726	0.0000
4	2	3	4	1	3	14531.9007	0.0002
4	2	2	4	1	3	14566.5932	0.0000
8	0	8	7	1	7	14615.1838	0.0005
3	2	2	3	1	2	14778.5820	0.0002
3	2	1	3	1	2	14790.1598	0.0004
4	1	3	3	0	3	14847.2529	-0.0005
2	2	1	2	1	1	14964.3265	0.0012
2	2	0	2	1	1	14966.6429	0.0008
2	2	1	2	1	2	15339.0784	0.0008
2	2	0	2	1	2	15341.3955	0.0012
3	2	2	3	1	3	15528.0440	0.0010
3	2	1	3	1	3	15539.6238	0.0032
7	1	7	6	1	6	15574.8801	0.0000
5	1	5	4	0	4	15590.9235	0.0008
4	2	3	4	1	4	15780.8216	-0.0013
4	2	2	4	1	4	15815.5133	-0.0023
7	0	7	6	0	6	15913.4253	0.0002
7	2	6	6	2	5	16023.0627	0.0002
7	3	5	6	3	4	16059.2767	-0.0008
7	3	4	6	3	3	16062.6500	0.0010
5	2	4	5	1	5	16098.0456	-0.0009
7	2	5	6	2	4	16150.1516	0.0004
5	2	3	5	1	5	16178.8179	-0.0008
7	1	6	6	1	5	16445.6382	0.0005
6	2	5	6	1	6	16480.4026	-0.0012
6	2	4	6	1	6	16641.3502	0.0009

7	2	6	7	1	7	16928.5868	0.0005
9	0	9	8	1	8	17185.0213	-0.0004
7	2	5	7	1	7	17216.6230	0.0026
8	2	7	8	1	8	17443.2188	0.0000
5	1	4	4	0	4	17463.7692	0.0003
6	1	6	5	0	5	17536.0897	0.0004
8	1	8	7	1	7	17789.5070	-0.0004
8	2	6	8	1	8	17919.2615	-0.0011
9	2	8	9	1	9	18024.7899	0.0004
8	0	8	7	0	7	18143.7141	0.0004
8	2	7	7	2	6	18304.1401	0.0001
8	3	6	7	3	5	18357.6030	-0.0002
8	3	5	7	3	4	18364.3308	0.0008
8	2	6	7	2	5	18492.1500	0.0002
8	1	7	7	1	6	18781.6763	0.0002
7	1	7	6	0	6	19441.9557	0.0001
2	2	1	1	1	0	19672.4731	0.0002
2	2	0	1	1	0	19674.7889	-0.0007
2	2	1	1	1	1	19797.3889	-0.0031
2	2	0	1	1	1	19799.7066	-0.0022

Table S31. Assigned transitions for the parent species of conformer VI of DAE.

J’	K_a’	K_c’	J”	K_a”	K_c”	ν_{obs} /MHz	$\nu_{obs - calc}$
2	1	1	2	0	2	6447.4081	0.0009
3	1	3	2	1	2	6453.4146	0.0000
3	1	2	3	0	3	6556.5148	0.0015
3	0	3	2	0	2	6558.3982	0.0005
3	1	2	2	1	1	6667.5037	-0.0001
4	1	3	4	0	4	6704.0837	0.0027

5	1	4	5	0	5	6891.8894	0.0020
6	1	5	6	0	6	7122.1280	0.0000
6	0	6	5	1	5	7278.8609	0.0025
7	1	6	7	0	7	7397.3864	-0.0019
8	1	7	8	0	8	7720.6022	-0.0015
9	1	8	9	0	9	8094.9997	0.0008
7	0	7	6	1	5	8152.5418	-0.0009
1	1	1	0	0	0	8490.9940	-0.0020
1	1	0	0	0	0	8562.3655	0.0018
4	1	4	3	1	3	8603.8338	0.0000
4	0	4	3	0	3	8741.6917	-0.0001
4	2	3	3	2	2	8747.3960	-0.0005
4	2	2	3	2	1	8753.4181	-0.0001
4	1	3	3	1	2	8889.2591	-0.0003
7	0	7	6	1	6	9650.8145	-0.0013
2	1	2	1	0	1	10606.5857	-0.0008
5	1	5	4	1	4	10753.6469	0.0003
2	1	1	1	0	1	10820.6862	-0.0005
5	0	5	4	0	4	10922.5607	0.0006
5	2	4	4	2	3	10933.4458	0.0002
5	4	2	4	4	1	10936.6903	0.0004
5	4	1	4	4	0	10936.6903	0.0003
5	3	3	4	3	2	10937.0563	-0.0016
5	3	2	4	3	1	10937.1255	0.0009
5	2	3	4	2	2	10945.4809	0.0008
5	1	4	4	1	3	11110.3663	-0.0001
8	0	8	7	1	7	12044.7144	0.0004
3	1	3	2	0	2	12686.7208	-0.0005
6	1	6	5	1	5	12902.7134	0.0002
6	0	6	5	0	5	13100.4106	0.0000
3	1	2	2	0	2	13114.9103	-0.0007

6	2	5	5	2	4	13118.9619	0.0005
6	4	3	5	4	2	13124.4010	0.0010
6	4	2	5	4	1	13124.4010	0.0005
6	3	4	5	3	3	13125.1793	-0.0001
6	3	3	5	3	2	13125.3572	-0.0001
6	2	4	5	2	3	13139.9945	0.0000
6	1	5	5	1	4	13330.6509	-0.0001
10	0	10	9	1	8	13675.7655	0.0002
9	0	9	8	1	8	14456.9286	-0.0012
4	1	4	3	0	3	14732.1581	0.0005
7	1	7	6	1	6	15050.9018	0.0000
7	0	7	6	0	6	15274.6712	0.0004
7	2	6	6	2	5	15303.8381	0.0002
7	4	4	6	4	3	15312.3114	-0.0010
7	4	3	6	4	2	15312.3114	-0.0027
7	3	5	6	3	4	15313.6620	0.0023
7	3	4	6	3	3	15314.0596	-0.0001
7	2	5	6	2	4	15337.4209	-0.0003
4	1	3	3	0	3	15445.7705	-0.0022
7	1	6	6	1	5	15549.9313	0.0001
5	1	5	4	0	4	16744.1120	-0.0002
10	0	10	9	1	9	16883.5294	0.0007
8	1	8	7	1	7	17198.0893	-0.0006
8	0	8	7	0	7	17444.7998	-0.0001
8	2	7	7	2	6	17487.9700	0.0007
8	4	4	7	4	3	17500.4636	-0.0018
8	4	5	7	4	4	17500.4636	0.0027
8	3	6	7	3	5	17502.5345	-0.0002
8	3	5	7	3	4	17503.3346	0.0002
8	2	6	7	2	5	17538.1875	-0.0003
8	1	7	7	1	6	17768.0158	0.0004

5	1	4	4	0	4	17814.4473	-0.0001
6	1	6	5	0	5	18724.2662	0.0008
11	0	11	10	1	10	19320.3424	0.0002
9	1	9	8	1	8	19344.1646	-0.0008
9	0	9	8	0	8	19610.3060	0.0001
9	2	8	8	2	7	19671.2489	-0.0011

Table S32. Assigned transitions for the parent species of conformer VII of DAE.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
1	1	1	0	0	0	6556.0985	0.0034
1	1	0	0	0	0	6707.6312	0.0005
4	0	4	3	1	2	7203.8999	-0.0003
6	1	5	5	2	3	7317.0830	-0.0001
4	0	4	3	1	3	8112.8981	-0.0010
3	1	3	2	1	2	8383.6364	-0.0001
3	0	3	2	0	2	8595.3452	0.0002
3	1	2	2	1	1	8838.0538	-0.0004
2	1	2	1	0	1	9275.8497	-0.0002
8	2	6	8	1	7	9583.2370	-0.0006
5	0	5	4	1	3	9690.8753	0.0006
2	1	1	1	0	1	9730.4320	0.0008
6	2	5	6	1	5	9730.6084	-0.0010
7	2	5	7	1	6	9788.5608	0.0013
6	2	4	6	1	5	10044.6220	-0.0002
5	2	4	5	1	4	10165.7799	0.0018
5	2	3	5	1	4	10324.3133	0.0002
7	1	6	6	2	4	10516.2061	-0.0007
4	2	3	4	1	3	10533.1644	-0.0001
4	2	2	4	1	3	10601.5023	-0.0031

3	2	2	3	1	2	10829.9153	0.0022
3	2	1	3	1	2	10852.7623	-0.0021
2	2	1	2	1	1	11054.0055	-0.0021
2	2	0	2	1	1	11058.5849	0.0005
4	1	4	3	1	3	11172.9052	0.0003
5	0	5	4	1	4	11205.2424	0.0012
4	0	4	3	0	3	11439.1323	0.0004
4	2	3	3	2	2	11481.5245	0.0005
4	3	2	3	3	1	11494.5330	0.0013
4	2	2	3	2	1	11527.0135	0.0000
4	1	3	3	1	2	11778.2722	-0.0002
3	1	3	2	0	2	11921.5770	-0.0006
4	2	3	4	1	4	12047.5280	-0.0030
6	0	6	5	1	4	12048.1505	0.0022
4	2	2	4	1	4	12115.8746	0.0026
5	2	4	5	1	5	12435.5001	0.0008
5	2	3	5	1	5	12594.0381	0.0038
3	1	2	2	0	2	12830.5757	-0.0008
6	2	5	6	1	6	12903.8352	0.0007
6	2	4	6	1	6	13217.8475	0.0002
8	1	7	7	2	5	13680.9129	-0.0004
5	1	5	4	1	4	13957.9085	0.0003
8	1	7	7	2	6	14237.8893	-0.0003
5	0	5	4	0	4	14265.2471	0.0003
6	0	6	5	1	5	14317.8708	0.0014
5	2	4	4	2	3	14345.8766	0.0001
5	3	3	4	3	2	14371.5552	-0.0008
5	3	2	4	3	1	14373.3634	-0.0015
5	2	3	4	2	2	14436.0710	0.0004
4	1	4	3	0	3	14499.1373	-0.0003
5	1	4	4	1	3	14713.2633	0.0003

6	1	6	5	1	5	16737.8923	-0.0002
9	1	8	8	2	6	16781.7465	0.0009
2	2	1	1	1	0	16948.0709	-0.0019
2	2	0	1	1	0	16952.6482	-0.0013
5	1	5	4	0	4	17017.9147	0.0008
6	0	6	5	0	5	17070.5367	0.0001
2	2	1	1	1	1	17099.6078	-0.0007
2	2	0	1	1	1	17104.1856	0.0004
6	2	5	5	2	4	17206.2269	-0.0008
6	3	4	5	3	3	17250.3838	-0.0006
6	3	3	5	3	2	17255.1923	-0.0015
6	2	4	5	2	3	17361.7061	0.0006
7	0	7	6	1	6	17433.2641	-0.0004
6	1	5	5	1	4	17641.3966	0.0002
5	1	4	4	0	4	19287.6332	-0.0018
6	1	6	5	0	5	19490.5615	0.0019
7	1	7	6	1	6	19512.2920	-0.0010
3	2	2	2	1	1	19667.9678	0.0005
3	2	1	2	1	1	19690.8191	0.0004
7	0	7	6	0	6	19853.2869	-0.0007

Table S33. Assigned transitions for the parent species of conformer VIII of DAE.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
1	1	1	0	0	0	6646.8503	0.0022
4	0	4	3	1	3	7414.1017	-0.0010
3	1	3	2	1	2	8325.7737	0.0000
3	0	3	2	0	2	8381.3697	0.0003
3	2	2	2	2	1	8382.7878	0.0029
3	2	1	2	2	0	8383.8922	0.0029

3	1	2	2	1	1	8438.9844	0.0011
7	1	6	6	2	5	8464.6614	-0.0021
2	1	2	1	0	1	9403.3226	-0.0003
5	0	5	4	1	4	10278.4113	-0.0005
8	2	6	8	1	7	11001.6727	0.0019
4	1	4	3	1	3	11100.6038	-0.0004
7	2	5	7	1	6	11126.4021	0.0010
4	0	4	3	0	3	11173.7456	0.0004
4	2	3	3	2	2	11176.7032	0.0001
4	3	2	3	3	1	11177.9862	-0.0011
4	3	1	3	3	0	11177.9924	-0.0025
4	2	2	3	2	1	11179.4629	0.0005
6	2	4	6	1	5	11240.8103	-0.0036
4	1	3	3	1	2	11251.5062	0.0010
5	2	3	5	1	4	11342.8155	0.0013
4	2	2	4	1	3	11430.5939	0.0013
3	2	1	3	1	2	11502.6380	0.0026
2	2	0	2	1	1	11557.7274	-0.0019
2	2	1	2	1	2	11670.6878	-0.0015
3	2	2	3	1	3	11727.6983	-0.0022
4	2	3	4	1	4	11803.7980	-0.0012
5	2	4	5	1	5	11899.0528	-0.0010
6	2	5	6	1	6	12013.5449	0.0006
3	1	3	2	0	2	12141.0114	-0.0002
7	2	6	7	1	7	12147.3616	0.0015
8	2	7	8	1	8	12300.5961	0.0003
6	0	6	5	1	5	13157.9195	0.0015
5	1	5	4	1	4	13875.0731	0.0000
5	0	5	4	0	4	13964.9140	0.0006
5	2	4	4	2	3	13970.3280	0.0004
5	3	3	4	3	2	13972.5259	-0.0016

5	4	2	4	4	1	13973.1172	0.0001
5	4	1	4	4	0	13973.1172	0.0000
5	2	3	4	2	2	13975.8406	0.0003
5	1	4	4	1	3	14063.6195	0.0009
4	1	4	3	0	3	14860.2437	-0.0030
7	0	7	6	1	6	16051.2786	-0.0006
6	1	6	5	1	5	16649.0951	0.0005
6	0	6	5	0	5	16754.5791	0.0000
6	2	5	5	2	4	16763.5853	0.0001
6	3	4	5	3	3	16767.0901	0.0006
6	3	3	5	3	2	16767.1600	-0.0001
6	4	3	5	4	2	16767.6371	-0.0026
6	4	2	5	4	1	16767.6371	-0.0027
6	2	4	5	2	3	16773.2178	0.0005
6	1	5	5	1	4	16875.2174	-0.0001
2	2	1	1	1	0	17183.6090	-0.0012
2	2	0	1	1	1	17221.6359	0.0012
5	1	5	4	0	4	17561.5751	0.0006
8	0	8	7	1	7	18956.9642	0.0023
9	3	6	9	2	7	19296.1521	-0.0003
7	3	4	7	2	5	19332.9776	-0.0002
6	3	3	6	2	4	19342.9300	0.0011
5	3	2	5	2	3	19348.9865	0.0005
4	3	1	4	2	2	19352.2723	0.0001
4	3	2	4	2	3	19356.4011	-0.0020
5	3	3	5	2	4	19358.6029	-0.0002
6	3	4	6	2	5	19362.1088	0.0013
7	3	5	7	2	6	19367.3740	-0.0005
7	1	7	6	1	6	19422.5868	-0.0005
7	0	7	6	0	6	19542.4557	-0.0002

Table S34. Assigned transitions for the parent species of conformer IX of DAE.

J'	K_a'	K_c'	J"	K_a"	K_c"	ν_{obs} /MHz	$\nu_{obs - calc}$
11	1	11	11	0	11	10225.7512	0.0012
10	1	10	10	0	10	10268.2169	0.0001
9	1	9	9	0	9	10306.9499	-0.0030
5	1	5	5	0	5	10423.9046	0.0011
4	1	4	4	0	4	10443.5053	0.0016
3	1	3	3	0	3	10459.2071	0.0010
2	1	2	2	0	2	10470.9964	0.0005
1	1	1	1	0	1	10478.8593	-0.0025
1	1	0	1	0	1	10486.7892	-0.0018
2	1	1	2	0	2	10494.7833	0.0006
3	1	2	3	0	3	10506.7797	0.0020
4	1	3	4	0	4	10522.7871	0.0020
5	1	4	5	0	5	10542.8159	-0.0011
6	1	5	6	0	6	10566.8900	0.0013
7	1	6	7	0	7	10595.0161	-0.0018
8	1	7	8	0	8	10627.2247	-0.0012
9	1	8	9	0	9	10663.5391	0.0022
10	1	9	10	0	10	10703.9764	-0.0009
11	1	10	11	0	11	10748.5778	0.0002
1	1	1	0	0	0	12340.2435	-0.0010
1	1	0	0	0	0	12348.1713	-0.0024
2	1	2	1	0	1	14193.7543	0.0011
2	1	1	1	0	1	14217.5403	0.0003
3	1	3	2	0	2	16043.3226	0.0008
3	1	2	2	0	2	16090.8929	-0.0004
4	1	4	3	0	3	17888.9539	0.0005
4	1	3	3	0	3	17968.2343	-0.0005
5	1	5	4	0	4	19730.6548	-0.0001

Appendix 5: Non-covalent interaction (NCI) isosurfaces for the conformers of DAS and DAE.

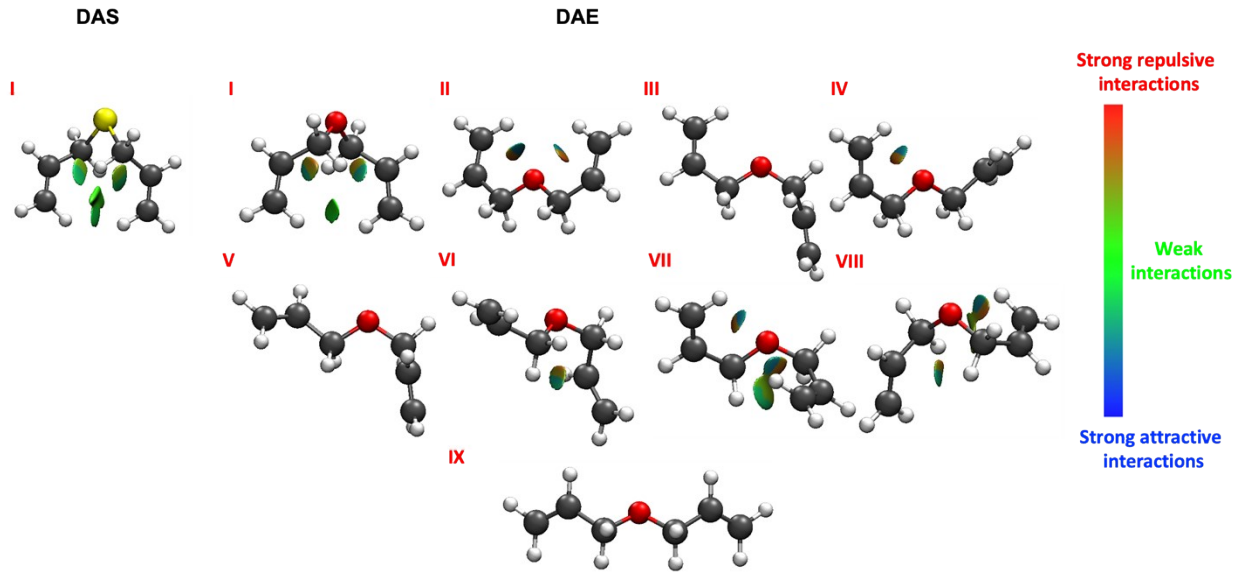

Figure S1. NCI isosurfaces (s = 0.05, color scale for -0.02 < ρ < 0.02 au) for the one and nine observed conformers for DAS and DAE respectively.

Appendix 6: Kraitchman coordinates of conformers I of DAS and DAE.

Table S35. Kraitchman coordinates of conformer I of DAS and DAE along with their uncertainties.

DAS	X	dX	Y	dY	Z	dZ
^{34}S	-0.00000	0.00000	-1.53264	0.00098	0.00000	0.00000
^{13}C1	1.11607	0.00134	-0.35177	0.00426	-0.82730	0.00181
^{13}C2	1.97373	0.00076	0.37652	0.00398	0.14761	0.01016
^{13}C3	1.93957	0.00077	1.71659	0.00087	0.28120	0.00533
^{13}C4	-1.11607	0.00134	-0.35177	0.00426	0.82730	0.00181
^{13}C5	-1.97373	0.00076	0.37652	0.00398	-0.14761	0.01016
^{13}C6	-1.93957	0.00077	1.71659	0.00087	-0.28120	0.00533

DAE	X	dX	Y	dY	Z	dZ
^{13}C1	0.93096	0.00161	-0.65621	0.00229	0.72648	0.00207
^{13}C2	1.89900	0.00079	0.06520	0.02301	-0.17530	0.00856
^{13}C3	2.10482	0.00071	1.38681	0.00108	-0.10214	0.01469
^{13}C4	-0.93096	0.00161	-0.65621	0.00229	-0.72648	0.00207
^{13}C5	-1.89900	0.00079	0.06520	0.02301	0.17530	0.00856
^{13}C6	-2.10482	0.00071	1.38681	0.00108	0.10214	0.01469

Appendix 7: Natural bond orbitals (NBO) results for conformer I of DAS and DAE.

Table S36. NBO results for conformers I of DAS and DAE and conformer XXIV and II of DAS and DAE, respectively.

DAS I		DAE I	
Interaction	E (kJmol)	Interaction	E(kJ/mol)
$LP_1(S) \rightarrow \sigma^*C_1–C_2$	2.4	$LP_1(O) \rightarrow \sigma^*C_1–C_2$	3.7
$LP_2(S) \rightarrow \sigma^*C_1–C_2$	15.6	$LP_2(O) \rightarrow \sigma^*C_1–C_2$	25.2
$LP_1(S) \rightarrow \sigma^*C_4–C_5$	2.4	$LP_1(O) \rightarrow \sigma^*C_4–C_5$	3.7
$LP_2(S) \rightarrow \sigma^*C_4–C_5$	15.6	$LP_2(O) \rightarrow \sigma^*C_4–C_5$	25.2
$LP_2(S) \rightarrow \pi^*C_4–C_5$	8.2	$LP_2(O) \rightarrow \pi^*C_4–C_5$	5.0
$LP_2(S) \rightarrow \pi^*C_5–C_6$	8.2	$LP_2(O) \rightarrow \pi^*C_5–C_6$	5.0
$LP_1(S) \rightarrow \sigma^*C_1–H$	13.7	$LP_1(O) \rightarrow \sigma^*C_1–H$	4.7
$LP_1(S) \rightarrow \sigma^*C_4–H$	13.7	$LP_1(O) \rightarrow \sigma^*C_4–H$	4.7

DAS XXIV		DAE II	
Interaction	E (kJmol)	Interaction	E(kJ/mol)
$LP_1(S) \rightarrow \sigma^*C_1–C_2$	-	$LP_1(O) \rightarrow \sigma^*C_1–C_2$	5.5
$LP_1(S) \rightarrow \sigma^*C_4–C_5$	-	$LP_1(O) \rightarrow \sigma^*C_4–C_5$	5.5
$LP_1(S) \rightarrow \sigma^*C_3–H$	-	$LP_1(O) \rightarrow \sigma^*C_3–H$	-
$LP_1(S) \rightarrow \sigma^*C_3–H'$	-	$LP_1(O) \rightarrow \sigma^*C_3–H'$	-
$LP_1(S) \rightarrow \sigma^*C_6–H$	-	$LP_1(O) \rightarrow \sigma^*C_6–H$	-
$LP_1(S) \rightarrow \sigma^*C_6–H'$	-	$LP_1(O) \rightarrow \sigma^*C_6–H'$	-
$LP_1(S) \rightarrow \sigma^*C_1–H$	4.1	$LP_1(O) \rightarrow \sigma^*C_1–H$	3.0
$LP_1(S) \rightarrow \sigma^*C_1–H'$	4.1	$LP_1(O) \rightarrow \sigma^*C_1–H'$	3.0
$LP_1(S) \rightarrow \sigma^*C_4–H$	4.1	$LP_1(O) \rightarrow \sigma^*C_4–H$	3.0
$LP_1(S) \rightarrow \sigma^*C_4–H'$	4.1	$LP_1(O) \rightarrow \sigma^*C_4–H'$	3.0
$LP_2(S) \rightarrow \pi^*C_2–C_3$	0.6	$LP_2(O) \rightarrow \pi^*C_2–C_3$	-
$LP_2(S) \rightarrow \pi^*C_5–C_6$	0.6	$LP_2(O) \rightarrow \pi^*C_5–C_6$	-

Appendix 8: Geometries of conformers XXIV of DAS and conformer II of DAE

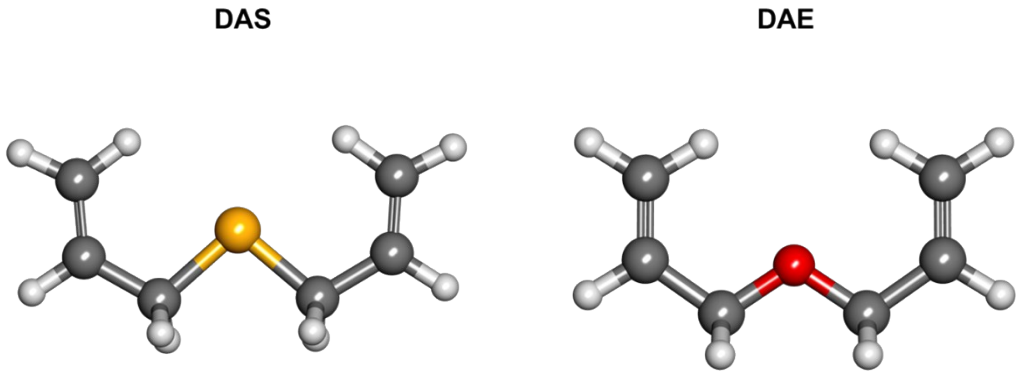

Figure S2. Structures of conformer XXIV and II of DAS and DAE, respectively.