Electronic Supporting Information for

Mechanistic Study of the Ring-Size Modulation in Michael–Dieckmann type Reactions of 2-Acylaminoacrylates with Ketene Diethyl Acetal

Submitted to **New Journal of Chemistry** by

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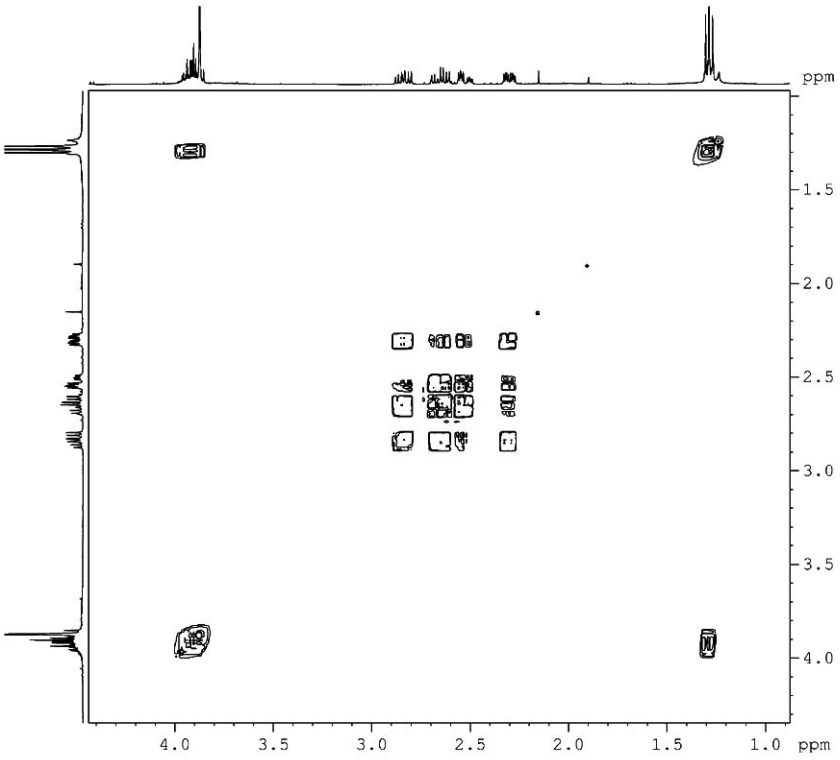
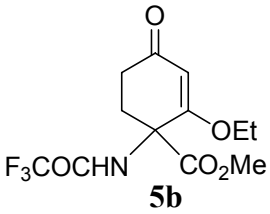
CONTENTS:

^{1}H and ^{13}C NMR spectra as well as COSY and HSQC correlations for compound 5b.

1-Trifluoroacetamido-2-ethoxy-4-oxocyclohex-2-ene-1-carboxylic acid methyl ester (5b)

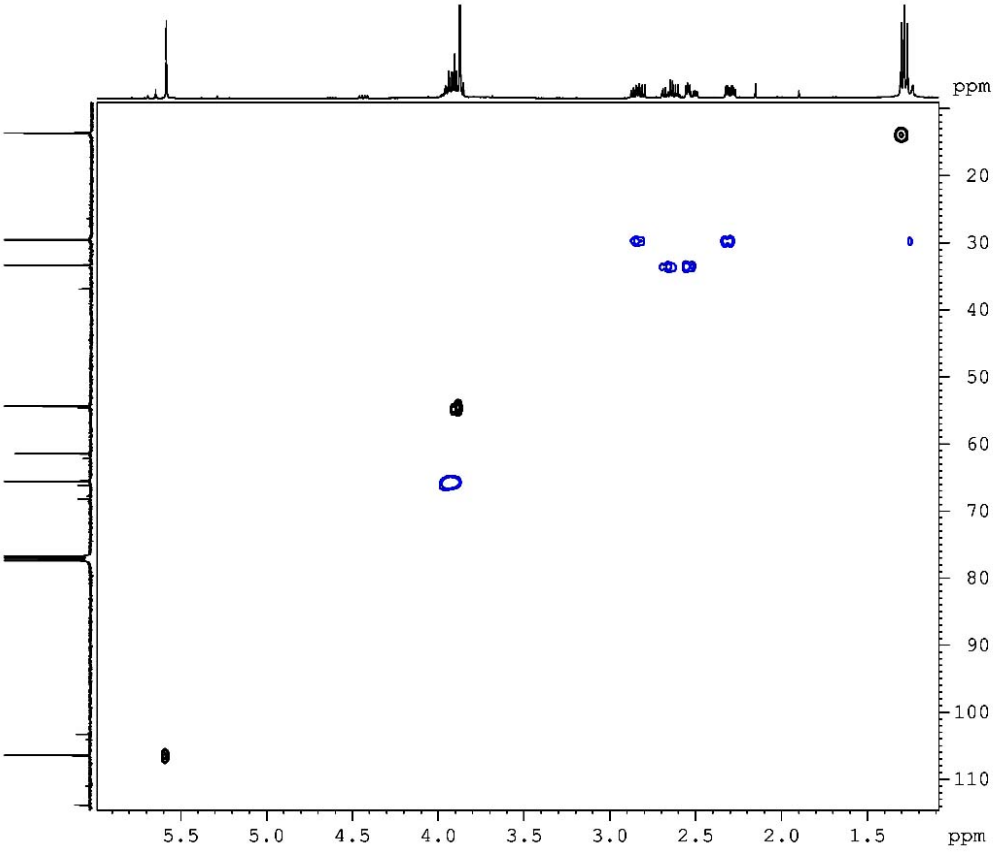
COSY





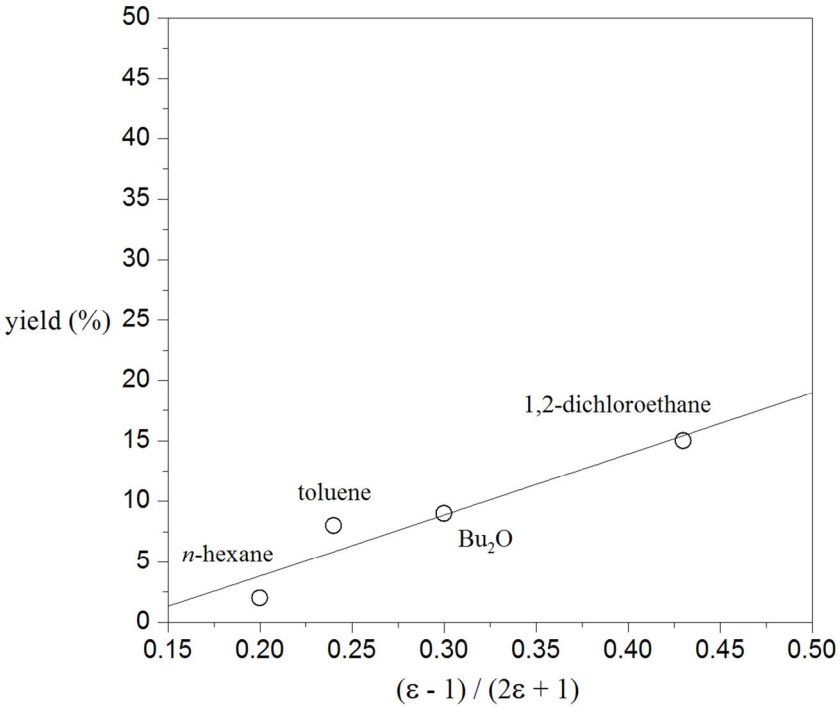
5b

HSQC Edited



Yield *vs.* solvent polarity plot obtained for the reaction between olefins 1 and 2a.

In an effort to obtain evidence for the existence of zwitterionic intermediates, we investigated the presence of significant solvent effects on the course of the reaction. When the reaction of olefin **1** with **2a** was carried out in various solvents of different polarity, we observed that the yield of the cycloaddition did depend on the solvent polarity, which is indicative of a polar reaction mechanism. For non-hydrogen-bond donor (non-HBD) solvents, the application of the simple electrostatic model of Kirkwood, Laidler and Eyring (J. G. Kirkwood, *J. Chem. Phys*., 1934, **2**, 351; C. J. F. Böttcher, *Theory of Electric Polarization*, Elsevier, New York, N. Y. 1952.), in which the dipolarity is represented as a function of the solvent dielectric permittivity ε, is enough to obtain a good linear relationship with the reaction yield, as shown in the next figure:

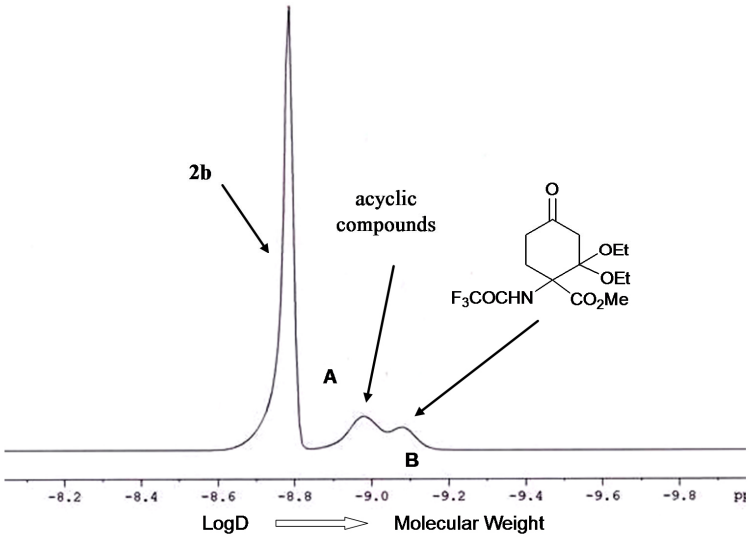


Materials balance on reaction of olefins 1 and 2b (DOSY and GC-MS experiments).

Important experimental efforts were made in order to perform a materials balance in the reactions carried out in this work. In this sense, it is clear that polymerization of olefin **2a** (S. Masuda, K. Minagawa, H. Ogawa and M. Tanaka, *Macromol. Chem. Phys.*, 2000, **201**, 1787) consumes almost all the reacting material when the cycloaddition is poorly produced, i. e. when carrying out the reaction with other solvents appart from *t*-butyl alcohol. This olefin has a high propensity to polymerize even in its pure form, so a 64% yield must be fairly appreciated, particularly for a thermal [2+2] cycloaddition.

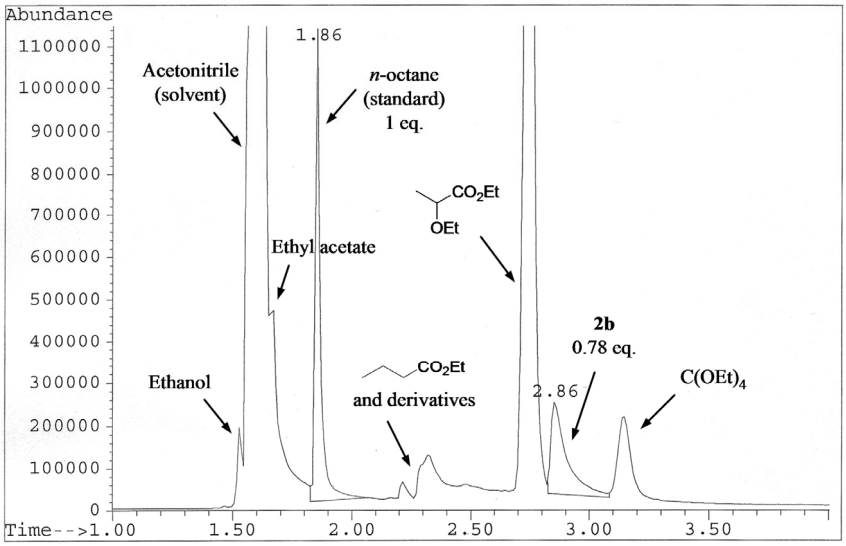
On the other hand, olefin **2b** appears to be much more stable with respect to polymerization than olefin **2a**. Therefore, and with the aim of evaluating its behaviour in solution, we have made modern NMR diffusion experiments (2D-DOSY) in order to study the crude mixture for reaction of **1** with **2b**. By the use of pulse gradient spin-echo (PGSE) NMR with LED-Bipolar pulse program (D. H. Wu, A. D. Chen and C. S. Johnson, *J. Magn. Reson. A*, 1995, **115**, 260), and applying the Stejskal-Tanner equation implemented into Bruker software, we have been able to estimate the diffusion coefficient (D), and therefore the molecular weight of some of the existing species. All experiments were made in $CDCl_3$ as a solvent and at 25 ºC with 535 L/h gas flow using Δ = 200 ms and δ = 2 ms. Gradient strength was first calibrated by measuring the self-diffusion coefficient of the residual HDO signal in a 100% D_2O sample at 298 K. Molecular weights were estimated by interpolating into a calibration curve made for known compounds.

In this sense, we observed a big amount of disturbing ketene diethyl acetal derivatives. By this reason, we focused on the analysis in the amide proton region, which corresponds exclusively to **2b**-derived compounds. The principal component of this mixture had a diffusion coefficient of D = 1.583 10^{-9} m^2/s, which was equal to that previously measured for the pure starting material. In the next figure, we show the projection along the diffusion dimension of the 2D-DOSY spectra for the crude mixture in the amide proton region.

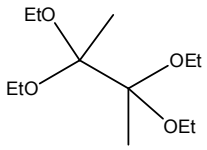


Some other signals were detected, being assigned as follow; signal **A** with molecular weight around 280 Dalton corresponding to acyclic compounds, and signal **B** with molecular weight around 350 Dalton and corresponding to a six-membered ring.

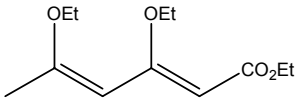
With the aim of quantitatively determining the remaining **2b**, the reaction was monitored by GC-MS with *n*-octane as an internal standard. The stationary phase employed was a 30 m × 0.25 mm × 0.25 μm SPB^{TM}-50 capillary column. The carrier gas was He with 1.0 mL/min flow. Injection was made in split mode (1:90) at 240 ºC, and detection at 270 ºC. The chromatograms were registered performing isocratic runs at 90 ºC and at different reaction times. These experiments clearly revealed the quick disappearance of **2b** within the first 10 minutes (22% conversion), but after the first 20 minutes the reaction stops. The amount of unreacted **2b** remains constant and the proportion of ketene diethyl acetal derivatives increases. Some of these species could be identified and are shown in the next chromatogram obtained at 40 minutes of reaction:



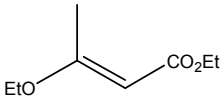
Some other ketene-derived compounds could be recognized at higher retention times (Rt):



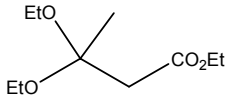
Rt = 4.21 min



Rt = 7.07 min



Rt = 8.56 min

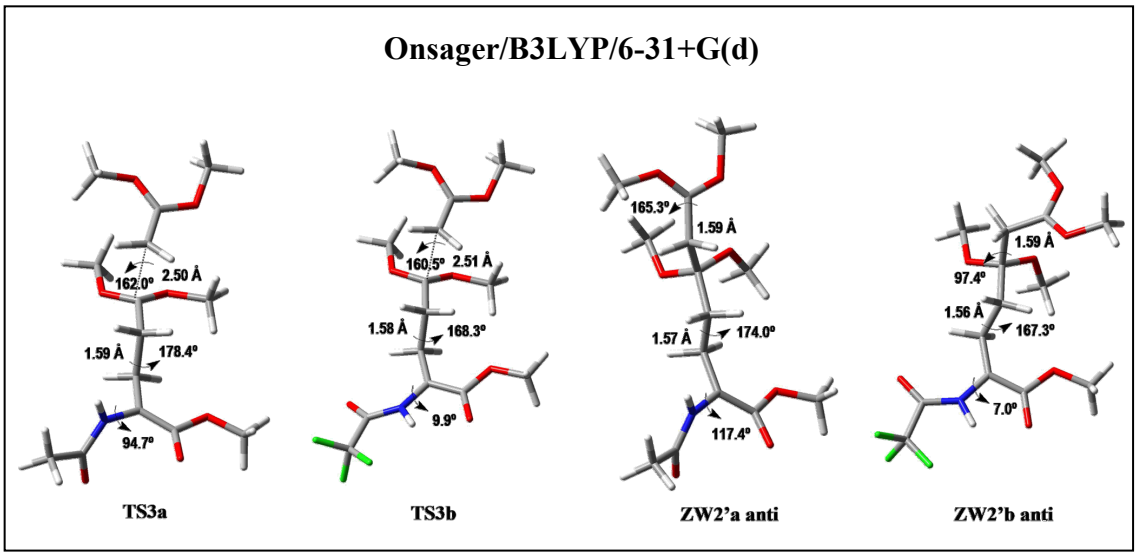


Rt = 9.32 min

Any other attempts to optimize the reaction by modifying the excess of donor olefin, temperature, solvent or rate of addition, resulted in a decrease of both the conversion and the global yield after column cromatography. This feature was surely due to the faster extinction of the reactive ketene diethyl acetal as compared with the two consecutive cycloadditions over **2b** required to form the six-membered products.

In conclusion, and in view of these experiments, we can assume that the materials balance are summarized with starting compound **2b** (78%), cyclohexanone prior to elimination together with its derived cyclohexenone **5b** (15-20 % overall) and some undefined acyclic intermediates (~5 %).

Optimized structures of the transition states (TS) and zwitterionic intermediates (ZW) considered in this work.



Tables for energies, enthalpies, free energies, and entropies of the structures considered in this work in vacuum and solution. Complete minimum energy paths in terms of $\Delta\Delta E$ and $\Delta\Delta G$.

Table S1. B3LYP/6-31+G* energies, enthalpies, free energies, and entropies of the structures considered in this work, calculated in vacuum.

Comp.	E_0	H	S	G	Lowest freq.
	(Hartree)[a]	(Hartree)[b]	(cal mol^{-1} K^{-1})[b]	(Hartree)[b]	(cm^{-1})
1'	-307.655898	-307.526576	86.2	-307.575517	100.7
2a	-514.512900	-514.345813	112.7	-514.409763	39.0
TS1a	-822.134804	-821.836859	157.0	-821.925980	154.5*i*
ZW1'a	-822.135084	-821.835741	157.7	-821.925252	27.8
3'a	-822.179107	-821.879374	150.0	-821.964529	49.6
	(Hartree)[a]	(Hartree)[c]	(cal mol^{-1} K^{-1})[c]	(Hartree)[c]	(cm^{-1})
1'	-307.655898	-307.530994	77.1	-307.562101	100.7
2b	-812.241525	-812.102985	108.7	-812.146833	23.2
TS1b	-1119.869147	-1119.604214	143.2	-1119.661993	254.6*i*
ZW1'b	-1119.869935	-1119.603549	142.4	-1119.661003	22.8
3'b	-1119.909347	-1119.642673	138.8	-1119.698648	21.5

[a] 1 Hartree = 627.5 Kcal mol^{-1}. [b] Thermal corrections at 356.15 K. [c] Thermal corrections at 253.15 K.

Table S2. Onsager[a]/B3LYP/6-31+G* energies, enthalpies, free energies, and entropies of the structures considered in this work, calculated in solution.

Comp.	E_0	H	S	G	Lowest freq.
	(Hartree)[b]	(Hartree)[c]	(cal mol^{-1} K^{-1})[c]	(Hartree)[c]	(cm^{-1})
1'	-307.656310	-307.527055	86.3	-307.576033	96.4
2a	-514.514367	-514.347328	112.8	-514.411357	37.0
TS1a anti	-822.142100	-821.844421	160.4	-821.935474	374.3*i*
TS1a gauche	-822.138514	-821.840628	157.9	-821.930241	271.3*i*
ZW1'a anti	-822.141332	-821.842062	161.2	-821.933579	20.0
ZW1'a gauche	-822.138920	-821.839649	159.6	-821.930231	26.2
TS2a	-822.135868	-821.837440	150.6	-821.922889	90.9*i*
3'a	-822.181376	-821.881738	150.7	-821.967257	52.0
TS3a	-1129.800612	-1129.371764	209.8	-1129.490857	171.7*i*
ZW2'a anti	-1129.819213	-1129.388671	205.1	-1129.505102	15.5
4'a	-1129.882605	-1129.449024	185.3	-1129.554176	37.7
5'a	-859.111247	-858.827626	150.8	-858.913199	32.5
	(Hartree)[b]	(Hartree)[d]	(cal mol^{-1} K^{-1})[d]	(Hartree)[d]	(cm^{-1})
1'	-307.656310	-307.531475	77.2	-307.562606	96.4
2b	-812.245553	-812.107168	108.8	-812.151052	22.0
TS1b anti	-1119.881284	-1119.616808	147.2	-1119.676187	368.0*i*
TS1b gauche	-1119.878143	-1119.613662	147.7	-1119.673253	364.6*i*
ZW1'b anti	-1119.888856	-1119.622772	147.5	-1119.682296	19.8
ZW1'b gauche	-1119.882267	-1119.615983	146.4	-1119.675049	17.9
TS2b	-1119.877909	-1119.612400	136.5	-1119.667451	43.8*i*
3'b	-1119.912885	-1119.646306	138.6	-1119.702238	23.8
TS3b	-1427.549520	-1427.158072	182.9	-1427.231866	159.3*i*
ZW2'b anti	-1427.563601	-1427.169934	179.7	-1427.242439	16.5

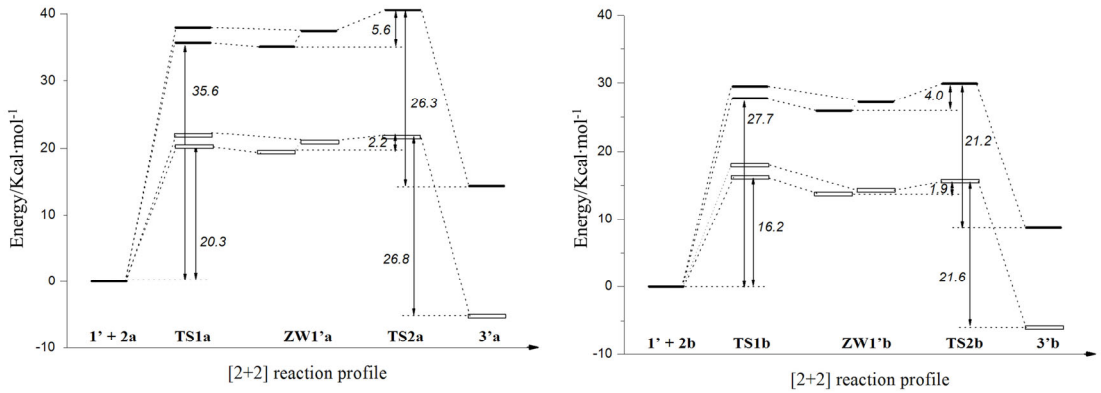
4'b	-1427.615532	-1427.219431	164.7	-1427.285879	21.4
5'b	-1156.841038	-1156.590272	138.1	-1156.645969	26.3

[a] Calculations in acetonitrile (ε = 36.64). [b] 1 Hartree = 627.5 Kcal mol^{-1}. [c] Thermal corrections at 356.15 K. [d] Thermal corrections at 253.15 K.

Table S3. PCM[a]/B3LYP/6-31+G* energies, enthalpies, free energies, and entropies of the structures considered in this work, calculated in solution.

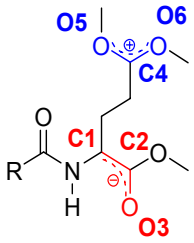
Comp.	E_0	H	S	G	Lowest freq.
	(Hartree)[b]	(Hartree)[c]	(cal mol^{-1} K^{-1})[c]	(Hartree)[c]	(cm^{-1})
1'	-307.659966	-307.530792	86.2	-307.579736	101.7
2a	-514.518943	-514.352176	112.9	-514.416275	38.0
TS1a anti	-822.147866	-821.850396	158.8	-821.940538	352.2*i*
TS1a gauche	-822.146682	-821.849207	156.6	-821.938065	346.2*i*
ZW1'a anti	-822.149216	-821.850158	160.7	-821.941356	16.8
ZW1'a gauche	-822.147991	-821.848952	157.7	-821.938441	27.0
TS2a	-822.145776	-821.847530	149.7	-821.932479	50.4*i*
3'a	-822.188580	-821.889244	150.1	-821.974453	52.9
4'a	-1129.889685	-1129.456589	186.3	-1129.562346	35.3
5'a	-859.121561	-858.838507	150.6	-858.923980	34.3
	(Hartree)[b]	(Hartree)[d]	(cal mol^{-1} K^{-1})[d]	(Hartree)[d]	(cm^{-1})
1'	-307.659966	-307.535223	77.1	-307.566321	101.7
2b	-812.246606	-812.108493	111.1	-812.153300	4.3
TS1b anti	-1119.882213	-1119.617999	146.1	-1119.676957	375.0*i*
TS1b gauche	-1119.881028	-1119.616933	145.2	-1119.675493	376.4*i*
ZW1'b anti	-1119.885856	-1119.619964	147.6	-1119.679498	10.1
ZW1'b gauche	-1119.886083	-1119.620164	144.6	-1119.678507	23.1
TS2b	-1119.883115	-1119.618100	136.9	-1119.673333	79.9*i*
3'b	-1119.917931	-1119.651683	138.5	-1119.707546	22.6
4'b	-1427.619676	-1427.224068	163.9	-1427.290193	24.8
5'b	-1156.849438	-1156.599218	136.4	-1156.654256	30.7

[a] IEF-PCM calculations in acetonitrile (ε = 36.64) using the RADII=UAHF keyword. [b] 1 Hartree = 627.5 Kcal mol^{-1}. [c] Thermal corrections at 356.15 K. [d] Thermal corrections at 253.15 K.



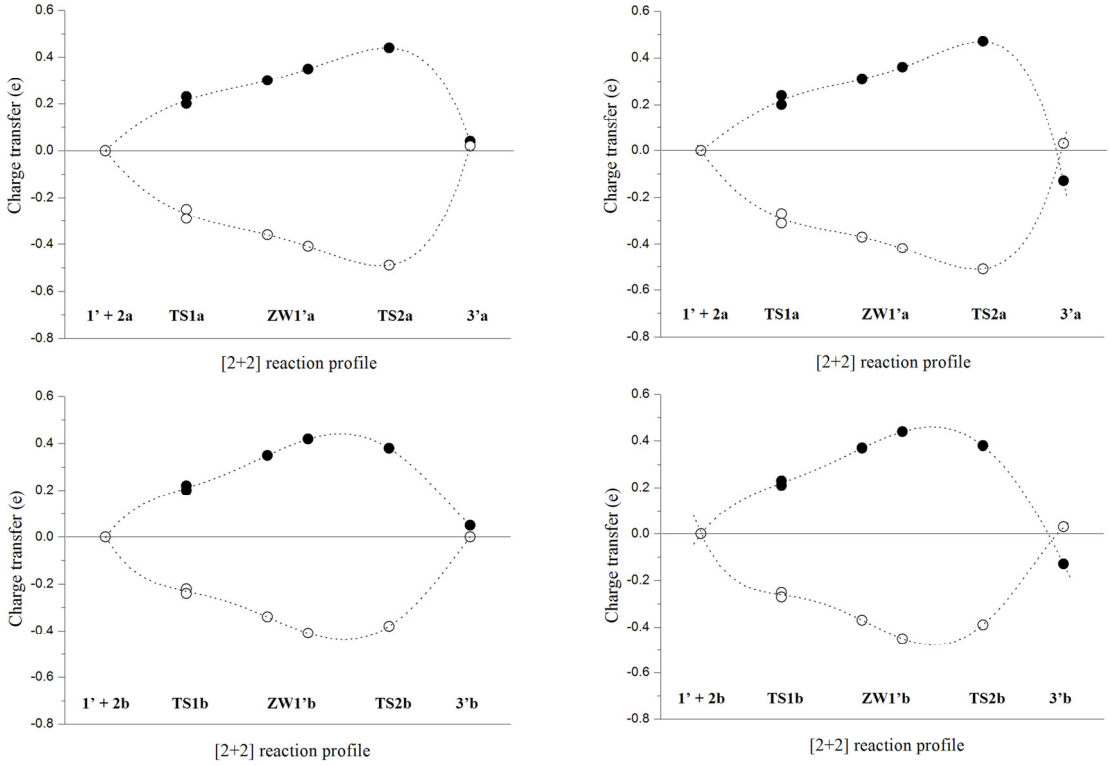
ΔΔ*E* (in white) *vs.* ΔΔ*G* (in black) along the [2+2] profile of olefins **2a** (left) and **2b** (right) calculated at the PCM/B3LYP/6-31+G(d) level. Numbers show the different activation barriers in Kcal·mol^{-1} for each step of the cycloaddition.

Definition of the donor and acceptor moieties considered in the charge transfer analyses and charge transfer plots



R = CH_3, CF_3

Comp.	C1		C2		O3		C4		O5		O6	
	AIM	NBO	AIM	NBO	AIM	NBO	AIM	NBO	AIM	NBO	AIM	NBO
1'							1.05	0.65	-1.12	-0.56	-1.12	-0.56
2a	0.38	0.03	1.60	0.80	-1.21	-0.64						
TS1a anti	0.34	-0.08	1.43	0.73	-1.26	-0.72	1.24	0.77	-1.11	-0.52	-1.1	-0.53
TS1a gauche	0.32	-0.10	1.42	0.72	-1.26	-0.73	1.27	0.79	-1.11	-0.51	-1.1	-0.52
ZW1'a anti	0.32	-0.11	1.36	0.70	-1.27	-0.75	1.33	0.83	-1.11	-0.49	-1.1	-0.51
ZW1'a gauche	0.28	-0.13	1.38	0.68	-1.28	-0.77	1.34	0.87	-1.11	-0.5	-1.1	-0.49
TS2	0.24	-0.19	1.32	0.67	-1.29	-0.79	1.48	0.94	-1.12	-0.47	-1.1	-0.48
3'a	0.38	0.00	1.63	0.85	-1.22	-0.62	1.03	0.61	-1.09	-0.61	-1.09	-0.61
2b	0.37	0.03	1.62	0.80	-1.21	-0.63						
TS1b anti	0.34	-0.09	1.47	0.74	-1.24	-0.70	1.24	0.77	-1.11	-0.52	-1.1	-0.53
TS1b gauche	0.33	-0.10	1.47	0.74	-1.25	-0.71	1.26	0.78	-1.11	-0.51	-1.1	-0.52
ZW1'b anti	0.31	-0.12	1.38	0.70	-1.27	-0.75	1.38	0.86	-1.11	-0.48	-1.1	-0.5
ZW1'b gauche	0.28	-0.17	1.36	0.69	-1.28	-0.77	1.45	0.92	-1.11	-0.49	-1.1	-0.47
TS2	0.25	-0.16	1.41	0.71	-1.26	-0.74	1.43	0.88	-1.12	-0.5	-1.11	-0.49
3'b	0.37	0.00	1.63	0.84	-1.21	-0.61	1.04	0.61	-1.09	-0.61	-1.08	-0.61



AIM (left) and NBO (righ) charge transfer along the [2+2] reaction profile of olefins **2a** (up) and **2b** (down) calculated at the PCM/B3LYP/6-31+G(d) level. The sum of the atomic charges at the acceptor olefin moiety (C1-C2-O3) is represented with white circles, and the sum of the atomic charges at the donor olefin moiety (C4-O5-O6) is represented with black circles.

Cartesian coordinates for the different conformations of the structures considered in this work.

Structure **1'** (B3LYP/6-31+G*)

C	0.00000200	1.42723900	-0.00005600
C	0.00000000	0.07937600	-0.00005000
O	-1.08294600	-0.73096900	0.00114800
C	-2.36689600	-0.11916000	-0.00037200
O	1.08294600	-0.73096900	-0.00133000
C	2.36689400	-0.11916100	0.00058500
H	-0.92266200	1.99044000	0.00143900
H	0.92266800	1.99043600	-0.00156800
H	-3.08414400	-0.94125000	-0.00097400
H	-2.50716000	0.49670600	-0.89749700
H	-2.50920600	0.49698300	0.89625500
H	3.08414200	-0.94125100	0.00149600
H	2.50684700	0.49678100	0.89770300
H	2.50951800	0.49690700	-0.89604700

Structure **1'** (Onsager/B3LYP/6-31+G*)

C	0.00001200	1.42519800	-0.00007400
C	-0.00000200	0.07838000	-0.00007100
O	1.08405200	-0.73305500	-0.00133300
C	2.36639000	-0.11661600	0.00060700
O	-1.08405700	-0.73305300	0.00110300
C	-2.36639600	-0.11660900	-0.00033100
H	-0.92197700	1.98941000	0.00140400
H	0.92201200	1.98939200	-0.00155600
H	-3.08676200	-0.93616700	-0.00091900
H	-2.50475400	0.49995000	-0.89709800
H	-2.50668200	0.50020000	0.89597700
H	3.08675300	-0.93617700	0.00156100
H	2.50435900	0.50001700	0.89738100
H	2.50707000	0.50011900	-0.89569600

Structure **1'** (PCM/B3LYP/6-31+G*)

C	-0.00003200	1.42738300	-0.00004300
C	-0.00000200	0.08065600	-0.00012000
O	1.08408700	-0.73218900	-0.00038900
C	2.37326600	-0.11817800	0.00022000
O	-1.08407100	-0.73220900	0.00028200
C	-2.37324700	-0.11819400	-0.00004000
H	-0.92346600	1.98940000	0.00039800
H	0.92337200	1.98944600	-0.00038300
H	-3.09026100	-0.94013700	-0.00017700
H	-2.51169800	0.49662800	-0.89713400
H	-2.51216300	0.49665700	0.89696700
H	3.09027600	-0.94012500	0.00038700
H	2.51158800	0.49654800	0.89740000
H	2.51232300	0.49676600	-0.89670100

Structure **2a** (B3LYP/6-31+G*)

C	-0.06852400	1.85090400	0.00005700
C	-0.09064700	0.50564900	0.00004100
N	1.01580400	-0.35853100	0.00006600
C	2.34985600	-0.01888900	-0.00003500
C	3.31123400	-1.19604700	0.00005900
C	-1.36464700	-0.28125200	-0.00000900
O	-2.47041600	0.47660600	0.00005900
C	-3.72355900	-0.23545700	-0.00002700
O	-1.38215600	-1.50323100	-0.00008200
O	2.74748600	1.14086600	-0.00014100
H	0.86376900	2.39812700	0.00006000
H	-1.00740900	2.39025600	0.00004500
H	-4.49058700	0.53886600	-0.00033300
H	-3.80344100	-0.86098600	0.89264100
H	-3.80310900	-0.86139100	-0.89243600
H	0.76109700	-1.34043700	0.00000500
H	3.95560600	-1.12240600	-0.88203500
H	2.81713800	-2.17271400	-0.00047100
H	3.95472000	-1.12298300	0.88285800

Structure **2a** (Onsager/B3LYP/6-31+G*)

C	-0.06979700	1.86274400	-0.00001500
C	-0.09264000	0.51852200	-0.00007700
N	1.01382400	-0.34693700	-0.00007600
C	2.34671800	-0.02073800	-0.00002200
C	3.29514300	-1.20975100	0.00009200
C	-1.36543800	-0.27689700	-0.00016200
O	-2.47183100	0.47255300	0.00002200
C	-3.72607100	-0.24712800	0.00013900
O	-1.36560100	-1.49845500	-0.00006900
O	2.76264300	1.13518700	0.00004300
H	0.86292000	2.40945600	0.00003200
H	-1.00914600	2.40157500	-0.00002000
H	-4.49543400	0.52416000	0.00013700
H	-3.80063100	-0.87201500	0.89307100
H	-3.80073600	-0.87213500	-0.89269800
H	0.74917800	-1.32727100	-0.00013700
H	3.93962500	-1.14450000	-0.88277700
H	2.78969200	-2.18033900	-0.00055200
H	3.93858700	-1.14517100	0.88377700

Structure **2a** (PCM/B3LYP/6-31+G*)

C	-0.07435100	1.84701800	0.00039900
C	-0.09047300	0.50179800	0.00025600
N	1.02008400	-0.35817500	0.00029100
C	2.35072200	-0.01955800	-0.00011500
C	3.31510300	-1.19082600	0.00012100
C	-1.36630300	-0.28623200	0.00012400
O	-2.46617600	0.47216500	-0.00002800
C	-3.72986800	-0.22826700	-0.00023600
O	-1.38020800	-1.50942100	-0.00011300
O	2.74600200	1.14636100	-0.00065500
H	0.85446900	2.39942300	0.00048300
H	-1.01503900	2.38324800	0.00038500
H	-4.48785300	0.55450700	-0.00041200
H	-3.81490500	-0.85035600	0.89409700
H	-3.81456200	-0.85040500	-0.89456700
H	0.77173500	-1.34247500	0.00039300
H	3.95887700	-1.11744000	-0.88283700
H	2.82281200	-2.16793900	-0.00029200
H	3.95795700	-1.11777800	0.88379100

Structure **TS0a** (B3LYP/6-31+G*)

C	-1.99439500	3.04264800	0.07312000
O	-1.30782400	1.85937600	-0.34671800
C	0.02824100	1.79876600	0.02170000
O	0.52353100	2.65957600	0.76588800
C	0.73973900	0.70984200	-0.55726400
N	2.10949400	0.67794700	-0.15442800
C	2.94709300	-0.38372900	-0.07956100
O	2.60424200	-1.55207200	-0.33720600
C	0.21049900	-0.16708200	-1.55803400
C	-0.40611400	-1.78057800	-1.08092800
C	-1.46364800	-1.58560500	-0.15707100
O	-2.68487300	-1.39105200	-0.62734800
C	-3.70181800	-0.84124000	0.23915200
O	-1.31687100	-1.33406500	1.12629900
C	-0.09542500	-1.71606400	1.81740500
C	4.37870600	-0.06541000	0.32108200
H	-0.75924400	-2.20269600	-2.02043200
H	0.48787900	-2.26605800	-0.70009800
H	-0.65801500	0.24982300	-2.06584400
H	0.95838300	-0.53199700	-2.26267700
H	2.42760900	1.56806400	0.21649300
H	-3.01227300	2.94284800	-0.31181400
H	-1.52207200	3.93801700	-0.34353200
H	-2.00367400	3.12748300	1.16427000
H	5.03701100	-0.24090100	-0.53787200
H	4.68688800	-0.75459100	1.11369900
H	4.52019000	0.96532100	0.66272900
H	0.78149800	-1.31798700	1.31332500
H	-0.05043800	-2.80837300	1.86905200
H	-0.20089500	-1.28747000	2.81318300

H	-3.39543200	0.15118600	0.57744100
H	-3.87414800	-1.50040100	1.09341600
H	-4.59263100	-0.78129500	-0.38526900

Structure **TS1a anti** (Onsager/B3LYP/6-31+G*)

C	-2.45906400	-0.48982900	0.39779400
C	-1.13285200	-0.34692400	0.84570400
C	0.01499600	-0.20618100	-0.68995200
C	1.32184300	0.17874900	-0.30484500
N	2.26480300	-0.73652300	0.24041500
C	1.73956400	1.53739100	-0.13477500
O	0.77653900	2.46185400	-0.46399900
C	1.16734700	3.83464700	-0.34859700
C	2.46019300	-2.04331500	-0.07797000
C	3.60179900	-2.72333800	0.67503300
O	-3.30858200	0.49379600	0.14225300
C	-3.02625900	1.83625800	0.59950500
O	-2.87619600	-1.68402600	0.01120400
C	-4.21589800	-1.84408900	-0.52405600
O	2.85315700	1.88763100	0.29200800
O	1.77106100	-2.68191600	-0.88150400
H	-0.72188000	-1.24261500	1.30207100
H	-0.91514900	0.56803400	1.38458000
H	-0.50958500	0.54176200	-1.27724200
H	-0.10167000	-1.22027200	-1.05999300
H	2.97442900	-0.27407900	0.79976700
H	0.29352600	4.41385400	-0.65249900
H	2.01448200	4.05424700	-1.00649700
H	1.44513700	4.07696000	0.68149300
H	-2.10229300	2.20440400	0.14603400
H	-2.95657300	1.84804400	1.69078400
H	-3.87930500	2.42882100	0.27199700
H	-4.33026000	-1.26565200	-1.44294400
H	-4.95668200	-1.52992300	0.21415700
H	-4.30293700	-2.91066800	-0.72498200
H	4.21585800	-2.03235100	1.26434700
H	4.23678500	-3.24376300	-0.05043700
H	3.18464200	-3.48007500	1.34971500

Structure **TS1a anti** (PCM/B3LYP/6-31+G*)

C	-2.42077000	-0.48977600	0.43538700
C	-1.09206500	-0.35583800	0.87840000
C	-0.00469400	-0.19442000	-0.66419500
C	1.31551400	0.18238400	-0.30507800
N	2.25735500	-0.74443000	0.22025100
C	1.72553000	1.54217900	-0.13321600
O	0.75559300	2.46154100	-0.46057500
C	1.14347200	3.83881500	-0.36696300
C	2.39690200	-2.06392300	-0.07666300
C	3.53995600	-2.77509900	0.62980600
O	-3.25954500	0.50304500	0.17382000
C	-2.93326000	1.84645200	0.59915400
O	-2.84237100	-1.68139500	0.03856300
C	-4.14269500	-1.81737300	-0.58547400
O	2.83817600	1.90237600	0.28861500
O	1.64438800	-2.67778600	-0.85061400
H	-0.67928200	-1.25897700	1.32025500
H	-0.87157800	0.54680200	1.43772000
H	-0.53468900	0.56076100	-1.23790600
H	-0.12707400	-1.20219900	-1.04823000
H	2.98646300	-0.30754100	0.77538800
H	0.26626900	4.41005100	-0.67635200
H	1.98599100	4.05229300	-1.03198700
H	1.42222200	4.09777000	0.65881400
H	-1.99898500	2.17489700	0.13713900
H	-2.85921900	1.88164800	1.68993700
H	-3.76647600	2.45879800	0.25637400
H	-4.18582700	-1.23083700	-1.50588500
H	-4.92695900	-1.49799700	0.10481800
H	-4.23188400	-2.88105600	-0.80285200
H	4.17101500	-2.10888200	1.22704500
H	4.16127000	-3.27735500	-0.11940900
H	3.12999400	-3.54981300	1.28795300

Structure **TS1a gauche** (Onsager/B3LYP/6-31+G*)

C	-1.70643000	3.12565800	-0.15133300
O	-1.03737300	1.94011000	-0.59480400
C	0.21682700	1.73529500	-0.06287200
O	0.69940400	2.51841300	0.77497400
C	0.87774100	0.57012700	-0.55471100
N	2.10187800	0.33234300	0.13546600
C	3.13530500	-0.48404900	-0.19819900
O	3.13696600	-1.25043800	-1.17288900
C	0.30000500	-0.37815700	-1.45186500
C	-0.49855600	-1.85090600	-0.71818400
C	-1.67351600	-1.46848300	-0.02545600
O	-2.79594000	-1.34678900	-0.70611200
C	-3.97010900	-0.78035600	-0.07219900
O	-1.72158000	-1.02345800	1.21577600
C	-0.62747300	-1.27927600	2.12926900
C	4.33401800	-0.42703600	0.74268000
H	-0.71922800	-2.45256600	-1.59706000
H	0.29026500	-2.27939300	-0.10635100
H	-0.50642900	0.03741300	-2.05194300
H	1.02480700	-0.93801900	-2.03810500
H	2.25045500	1.01564700	0.87346700
H	-2.66452800	3.13275000	-0.67513500
H	-1.12874600	4.01956900	-0.40742400
H	-1.86374500	3.10687100	0.93144400
H	5.22943000	-0.19183100	0.15613800
H	4.48743200	-1.41629200	1.18869200
H	4.23069100	0.30861000	1.54786100
H	0.29388600	-0.82317800	1.76509800
H	-0.51095100	-2.35929800	2.26013200
H	-0.93682900	-0.81732200	3.06592500
H	-3.77002400	0.25221000	0.22132500
H	-4.25541200	-1.37635800	0.79720300
H	-4.74290400	-0.82482100	-0.83788600

Structure **TS1a gauche** (PCM/B3LYP/6-31+G*)

C	-1.82339800	3.06676600	-0.13343900
O	-1.11131500	1.90156500	-0.56709400
C	0.13909100	1.72667800	-0.02040600
O	0.57933700	2.50651400	0.84573900
C	0.85007100	0.60059400	-0.53591000
N	2.07775800	0.37966000	0.15525400
C	3.13889100	-0.39013400	-0.20349900
O	3.15935900	-1.10990200	-1.21638400
C	0.31409700	-0.32522600	-1.47335500
C	-0.48082000	-1.88475700	-0.79315700
C	-1.62400600	-1.51544300	-0.05744600
O	-2.76710600	-1.34388000	-0.69903900
C	-3.89130600	-0.74039500	-0.01498800
O	-1.62977000	-1.12481200	1.20296600
C	-0.51206200	-1.44241700	2.06982400
C	4.33035800	-0.33988800	0.73989900
H	-0.71517200	-2.41657600	-1.71247800
H	0.32845000	-2.33588900	-0.22704900
H	-0.50616300	0.07339600	-2.06453900
H	1.05130500	-0.86699300	-2.05823200
H	2.20241500	1.02154600	0.93281600
H	-2.77065900	3.04743100	-0.67589600
H	-1.26892600	3.97802000	-0.37902000
H	-2.00257800	3.03847400	0.94578400
H	5.21939700	-0.04475000	0.17171700
H	4.51604900	-1.34350600	1.13900100
H	4.20041600	0.35171800	1.57864900
H	0.40196500	-0.97080300	1.70686500
H	-0.39751900	-2.52860000	2.13055300
H	-0.79102100	-1.03547200	3.04108700
H	-3.63565300	0.27542900	0.29380200
H	-4.17613500	-1.34197900	0.85116700
H	-4.69000300	-0.72962200	-0.75565200

Structure **ZW1'a** (B3LYP/6-31+G*)

C	-2.02013200	2.96873400	0.05047900
O	-1.32672500	1.78485800	-0.35034300
C	0.02743500	1.75458700	-0.00115600
O	0.50891900	2.63920300	0.72909400
C	0.73484200	0.67282300	-0.57038600
N	2.12502800	0.67025600	-0.23803400
C	2.93288000	-0.39582700	-0.04888500
O	2.54145900	-1.57845700	-0.13123500
C	0.19445800	-0.22994800	-1.57654900

C	-0.37707100	-1.73908400	-1.09276500
C	-1.43826200	-1.54226500	-0.14094700
O	-2.66366900	-1.43109900	-0.60870500
C	-3.70826600	-0.90513100	0.24489000
O	-1.29615400	-1.24459800	1.11901700
C	-0.05683700	-1.45281300	1.86685200
C	4.39084200	-0.08413600	0.24352800
H	-0.76682400	-2.22280200	-1.98955700
H	0.49761200	-2.25522200	-0.70217000
H	-0.65328600	0.21687500	-2.09997000
H	0.95466300	-0.53953100	-2.29937100
H	2.48171700	1.58747700	0.01220400
H	-3.04445900	2.84784100	-0.31249100
H	-1.56910600	3.86021600	-0.39777700
H	-2.01169600	3.08514400	1.13903800
H	5.00491700	-0.40570900	-0.60589900
H	4.70984900	-0.66547100	1.11455700
H	4.58214900	0.97824400	0.42804000
H	0.80182600	-1.56695600	1.20685600
H	-0.21731200	-2.34178200	2.48364200
H	0.05403300	-0.56487900	2.48762600
H	-3.44159000	0.10677500	0.55666100
H	-3.84896800	-1.55158800	1.11412500
H	-4.59870700	-0.90133100	-0.38227100

Structure **ZW1'a anti** (Onsager/B3LYP/6-31+G*)

C	-2.42036700	-0.43647800	0.37735900
C	-1.03355600	-0.25832400	0.74747300
C	-0.06964500	-0.17304700	-0.62874700
C	1.30698800	0.17638500	-0.29333900
N	2.19071300	-0.78957600	0.26491300
C	1.76533700	1.49977300	-0.11145400
O	0.81363400	2.46810500	-0.41865900
C	1.26114500	3.82001600	-0.32180800
C	2.36487100	-2.08480400	-0.10605000
C	3.43755200	-2.84046900	0.67610100
O	-3.27627200	0.52623900	0.12613000
C	-2.98551800	1.90349900	0.49021900
O	-2.82740400	-1.64109800	0.06893300
C	-4.18087400	-1.85611700	-0.43154400
O	2.89432000	1.83097100	0.31054800
O	1.69945900	-2.66204900	-0.97606300
H	-0.67027600	-1.12197800	1.30547500
H	-0.87339800	0.66144800	1.30644100
H	-0.51471500	0.58679400	-1.27238300
H	-0.15956600	-1.15866100	-1.08773900
H	2.89295900	-0.37579500	0.87085300
H	0.40099400	4.43625000	-0.59384700
H	2.09107200	4.00961300	-1.01201500
H	1.58941600	4.05704800	0.69528300
H	-2.05922700	2.23180200	0.01416600
H	-2.92180100	1.98413900	1.57805000
H	-3.83830700	2.46991700	0.11998700
H	-4.31841300	-1.32213600	-1.37319200
H	-4.90671500	-1.51816900	0.31012900
H	-4.24647200	-2.93229900	-0.57773500
H	2.95875300	-3.59765100	1.30836300
H	4.08154700	-3.36790000	-0.03644900
H	4.05366600	-2.19534300	1.31384700

Structure **ZW1'a anti** (PCM/B3LYP/6-31+G*)

C	-2.37945100	-0.46942000	0.40687000
C	-0.99231300	-0.30948400	0.77631100
C	-0.07314000	-0.18436500	-0.61859400
C	1.30641400	0.18756700	-0.31025300
N	2.20295000	-0.76792300	0.24740700
C	1.72349200	1.52346700	-0.12228700
O	0.74748200	2.46308900	-0.43897900
C	1.15324100	3.83178500	-0.35193100
C	2.35567800	-2.07154100	-0.09956200
C	3.42047400	-2.83532700	0.67195900
O	-3.22623700	0.50586800	0.17956000
C	-2.89437100	1.87514300	0.54378200
O	-2.79160600	-1.66352700	0.06203000
C	-4.12095400	-1.84592700	-0.50250700
O	2.83942700	1.89074000	0.30731200
O	1.66397800	-2.63900900	-0.96449900
H	-0.62398500	-1.19201900	1.30142700
H	-0.82274000	0.58916300	1.36628500
H	-0.54666300	0.57294600	-1.24454200
H	-0.15624800	-1.16589300	-1.08624100
H	2.89513800	-0.36651500	0.87317300
H	0.27714500	4.41695300	-0.64042700
H	1.98315300	4.04078400	-1.03529700
H	1.45965400	4.09004700	0.66660200
H	-1.96806000	2.18113500	0.05354900
H	-2.80869500	1.94908200	1.63071000
H	-3.73730300	2.46432700	0.18623600
H	-4.20926500	-1.28206400	-1.43315600
H	-4.87478000	-1.52138800	0.21751100
H	-4.19232800	-2.91650400	-0.68647400
H	2.94005600	-3.59385900	1.30139100
H	4.06507800	-3.36150200	-0.04001800
H	4.04041100	-2.19790700	1.31129300

Structure **ZW1'a gauche** (Onsager/B3LYP/6-31+G*)

C	-1.67819400	-1.42092400	0.00258400
C	-0.46329800	-1.79690800	-0.67541900
C	0.27527500	-0.45734200	-1.41532600
C	0.87857600	0.53970900	-0.54799200
N	2.09726100	0.28918800	0.15113300
C	0.23717200	1.71313900	-0.08763100
O	-1.02839600	1.91151200	-0.61979000
C	-1.68445500	3.11252800	-0.20681200
C	3.14527200	-0.49862400	-0.19945500
C	4.32888800	-0.46739200	0.76268300
O	-1.75927800	-0.95820800	1.22496100
C	-0.66541800	-1.12149500	2.16889800
O	-2.78199400	-1.36722300	-0.69782700
C	-4.00299000	-0.84469800	-0.10282100
O	0.72010300	2.51993000	0.73514800
O	3.17227700	-1.22933800	-1.20305500
H	-0.69436000	-2.48110000	-1.49220800
H	0.28650500	-2.22955700	-0.01423400
H	-0.50091400	-0.02035000	-2.04386300
H	1.01597300	-0.97952400	-2.02215400
H	2.23950700	0.96433000	0.89848100
H	-2.64574600	3.11468900	-0.72576200
H	-1.10216100	3.99592700	-0.48966300
H	-1.83815500	3.12787800	0.87690400
H	5.23589500	-0.22938200	0.19501400
H	4.46844100	-1.46461800	1.19610900
H	4.21668600	0.25526000	1.57874400
H	0.24778200	-0.67332700	1.77853700
H	-0.53614400	-2.18685600	2.37900200
H	-0.99925000	-0.59734600	3.06293700
H	-3.85568500	0.20203700	0.16891300
H	-4.27378700	-1.43693100	0.77316500
H	-4.75207500	-0.94679400	-0.88560000

Structure **ZW1'a gauche** (PCM/B3LYP/6-31+G*)

C	-1.58743100	-1.46333300	-0.02370200
C	-0.38652600	-1.79513000	-0.76161200
C	0.27758100	-0.42794700	-1.43948600
C	0.83171900	0.58041200	-0.53330800
N	2.06153100	0.36138200	0.16249200
C	0.12353100	1.69409200	-0.04577400
O	-1.15505600	1.83066100	-0.58162900
C	-1.86727500	3.00586900	-0.18979600
C	3.14136300	-0.37061100	-0.20855400
C	4.32137300	-0.33095000	0.75059100
O	-1.63198800	-1.08370400	1.22161000
C	-0.49833100	-1.27979200	2.11975500
O	-2.70690800	-1.37311300	-0.68827700
C	-3.89548000	-0.83784400	-0.04171700
O	0.54522000	2.51479500	0.80487200
O	3.19020900	-1.05946200	-1.24578300
H	-0.64050600	-2.45006000	-1.59737400
H	0.37793800	-2.25903900	-0.13805700
H	-0.50830200	-0.00025500	-2.06354100
H	1.04851800	-0.87719600	-2.06695000
H	2.17424600	0.99671000	0.94799000
H	-2.82331200	2.95927700	-0.71672000
H	-1.32631900	3.91246700	-0.48174000

H	-2.03374500	3.02808200	0.89223700
H	5.21673600	-0.02475700	0.19820700
H	4.50725400	-1.33889500	1.13949500
H	4.17830600	0.34810900	1.59774900
H	0.38667600	-0.78147200	1.72676600
H	-0.33576100	-2.35268200	2.24977200
H	-0.81638600	-0.82447400	3.05617600
H	-3.70321300	0.19074500	0.26815900
H	-4.16262200	-1.45822500	0.81594700
H	-4.66517800	-0.88000800	-0.81029300

Structure **TS2a** (Onsager/B3LYP/6-31+G*)

C	2.22976900	3.07676000	-0.24524700
O	1.51541900	1.93981100	0.23053000
C	0.17175800	1.87527600	-0.15412400
O	-0.30150000	2.75610100	-0.91108100
C	-0.53262500	0.78341400	0.38186500
C	1.23600000	-1.58328100	0.29465100
O	2.40990600	-1.10155100	0.52031800
C	3.42571700	-1.08230400	-0.52813800
C	0.25152200	-1.47162400	1.40413300
C	-0.09935600	0.03928500	1.61766900
O	1.05504600	-2.13371800	-0.85518200
C	-0.21131700	-2.77391600	-1.24186800
N	-1.93435500	0.88849100	0.08928300
C	-2.84730300	-0.09376500	-0.00170900
O	-2.60586800	-1.29954800	0.22627200
H	0.72096400	-1.89099500	2.30493200
H	-0.65856800	-2.02037600	1.16702000
H	0.78110800	0.53148300	2.04311300
H	-0.88821500	0.05124800	2.38492000
H	-2.18029300	1.80390700	-0.28198600
H	3.24929200	2.96450200	0.13363700
H	1.79327900	4.00946700	0.13115600
H	2.23526900	3.11548800	-1.34001600
H	-0.12584900	-2.88339900	-2.32133300
H	-1.05523900	-2.14469200	-0.95041900
H	-0.25034600	-3.75184100	-0.75847000
H	3.06413200	-0.47023200	-1.35501100
H	3.63778000	-2.10207700	-0.85247600
H	4.29359400	-0.63167100	-0.05218100
C	-4.25715200	0.33773400	-0.38346100
H	-4.32882000	1.39724400	-0.65582300
H	-4.59653000	-0.27481400	-1.22620300
H	-4.93717100	0.14309300	0.45469000

Structure **TS2a** (PCM/B3LYP/6-31+G*)

C	2.49471100	2.81965900	-0.19936500
O	1.64689000	1.79867800	0.32219400
C	0.33251700	1.79925400	-0.15603900
O	-0.01778600	2.66114800	-1.00492800
C	-0.48741700	0.80651900	0.39730500
C	1.10816100	-1.60835600	0.29076200
O	2.29880400	-1.15922500	0.49569700
C	3.28877200	-1.16175700	-0.57641100
C	0.14699800	-1.47663100	1.42267500
C	-0.14450300	0.03783400	1.65175500
O	0.89667600	-2.16474700	-0.85160700
C	-0.39598500	-2.75463300	-1.22274600
N	-1.86568800	0.99875900	0.04714900
C	-2.85808900	0.09230200	-0.00988500
O	-2.70780100	-1.11966800	0.27237500
H	0.61347500	-1.93218100	2.30831800
H	-0.78248000	-1.99280600	1.18977400
H	0.73828300	0.48786800	2.11698300
H	-0.96271500	0.08679400	2.38411600
H	-2.05515500	1.92327500	-0.33180300
H	3.46181200	2.67806700	0.29020600
H	2.10721400	3.81902200	0.02737100
H	2.60942800	2.72910400	-1.28553400
H	-0.32696500	-2.87486100	-2.30256700
H	-1.20945400	-2.08767700	-0.92997500
H	-0.47315700	-3.72590800	-0.73010400
H	2.90838300	-0.57370000	-1.41239600
H	3.49411700	-2.18987500	-0.87922400
H	4.16666900	-0.69662600	-0.13324100
C	-4.22263100	0.61893000	-0.42244500
H	-4.21050900	1.66947600	-0.73176600
H	-4.60500400	0.00796700	-1.24764300
H	-4.92359100	0.51253300	0.41396600

Structure **3'a** (B3LYP/6-31+G*)

C	3.55549000	0.01616400	0.18888800
O	2.17603100	0.30238500	-0.04705000
C	1.26923700	-0.71065600	0.30219700
O	1.39789900	-1.85342500	-0.50164300
C	1.45702900	-1.61319300	-1.92118300
C	1.19026600	-1.02407600	1.81323200
C	0.05958400	0.03242700	1.94069200
C	-0.17014800	-0.04349900	0.40275400
N	-1.16190300	-1.03770200	0.03887100
C	-2.50219000	-0.79612100	0.14935200
C	-3.42037600	-1.89714100	-0.35229500
C	-0.37496100	1.23262100	-0.41935400
O	-0.21466200	2.34940800	0.30353400
C	-0.38434700	3.58638000	-0.41280600
O	-0.62145500	1.22160900	-1.60927000
O	-2.93376500	0.25477600	0.61820400
H	0.43268400	1.01255800	2.23982200
H	-0.80968400	-0.23110600	2.54505700
H	2.10229100	-0.86349200	2.39368200
H	3.78624100	0.00864700	1.26137800
H	0.83868800	-2.04608500	1.97706300
H	4.11323200	0.82341700	-0.29054900
H	-4.19681000	-2.07898100	0.39634400
H	0.34583300	3.65785500	-1.22337600
H	3.84716600	-0.94495200	-0.25000000
H	-1.39505900	3.64484500	-0.82463300
H	-0.82662500	-1.88329600	-0.40535700
H	-3.91531400	-1.55015100	-1.26627900
H	-2.90009800	-2.83603800	-0.56891400
H	-0.22203200	4.37166400	0.32601800
H	2.40961000	-1.15325700	-2.20294700
H	0.63792300	-0.96546200	-2.25111800
H	1.37538800	-2.59771200	-2.38735100

Structure **3'a** (Onsager/B3LYP/6-31+G*)

C	-3.59420100	0.19645000	-0.14383200
O	-2.18818300	0.46322300	-0.10453200
C	-1.35136500	-0.65734400	-0.10121500
C	0.11031100	-0.18024700	-0.53939500
N	1.08537000	-0.96709300	0.19130300
C	2.42539600	-0.90229500	-0.04829800
C	3.29751900	-1.79659300	0.81714800
C	-1.40498600	-1.54196100	-1.36856100
C	-0.20879000	-0.74407000	-1.95208000
O	-1.44423500	-1.40658800	1.08200000
C	-1.44183600	-0.65894800	2.31288200
C	0.38096600	1.32352700	-0.46805700
O	0.76742900	1.70058100	0.76815300
C	1.01489200	3.10580000	0.94388900
O	0.22215600	2.09511000	-1.38892100
O	2.90217700	-0.15679700	-0.90462300
H	-3.90303400	-0.16275300	-1.13280300
H	-4.08348300	1.15095600	0.05931000
H	-2.34237200	-1.52485700	-1.92993500
H	-3.88620100	-0.53719200	0.61549000
H	-0.51522800	0.05713500	-2.62713900
H	-1.15664700	-2.57853800	-1.12551100
H	0.60186600	-1.31823600	-2.40473500
H	-2.35877600	-0.07249000	2.42134700
H	0.10725000	3.67949100	0.73709600
H	-1.39157700	-1.40621600	3.10721500
H	-0.57846700	0.01281000	2.36861600
H	1.81477700	3.43308900	0.27400100
H	0.72035800	-1.58825400	0.90388000
H	1.31358600	3.21971500	1.98659500
H	2.72985100	-2.47090000	1.46620300
H	3.94960400	-2.38942300	0.16826000
H	3.93872100	-1.16483300	1.44149500

Structure **3'a** (PCM/B3LYP/6-31+G*)

C	-3.59499200	0.18889300	-0.16161000
O	-2.18766400	0.45538500	-0.12499400

C	-1.35147600	-0.66600400	-0.08744700
O	-1.44905900	-1.37963400	1.11876300
C	-1.42546500	-0.59155300	2.32501500
C	0.10950100	-0.19801600	-0.53380500
C	0.37956200	1.30735800	-0.48657900
O	0.23527800	2.06020000	-1.42879700
C	-1.40054400	-1.58415000	-1.33012500
C	-0.20969000	-0.79402300	-1.93400200
N	1.09039700	-0.96628600	0.21025900
C	2.42653100	-0.89283200	-0.03496000
O	2.88820400	-0.13923900	-0.89774600
C	3.31480400	-1.77307400	0.82353700
O	0.74644200	1.70862600	0.74259100
C	0.99391200	3.11886900	0.90669200
H	-3.89656700	-0.22551200	-1.13067300
H	-4.08370400	1.15426400	-0.01612400
H	-2.33653800	-1.58895000	-1.89373700
H	-3.89347300	-0.49904400	0.63722100
H	-0.52540000	-0.01319600	-2.62824900
H	-1.14046400	-2.61201200	-1.06271800
H	0.60003800	-1.37708100	-2.37696800
H	-2.33959200	0.00086600	2.42686300
H	0.08834900	3.69007300	0.68563600
H	-1.36196400	-1.31167700	3.14344400
H	-0.55944600	0.07794900	2.34446000
H	1.80225800	3.43874900	0.24400200
H	0.73349800	-1.60066000	0.91580100
H	1.28156400	3.24239700	1.95096500
H	2.75803200	-2.44014800	1.48898500
H	3.95610800	-2.37409800	0.17092000
H	3.96605200	-1.13343000	1.42952400

Structure **TS3a** (Onsager/B3LYP/6-31+G*)

C	2.65597400	-0.39737600	-1.23796700
C	3.94801300	-0.08161900	-0.84392900
C	-2.78410000	0.03127500	0.01142800
C	-1.49793500	-0.08389200	0.77247400
C	-0.19588200	-0.17480700	-0.14509900
C	1.05804900	-0.24860400	0.67435100
N	-3.36613500	-1.17830000	-0.49318500
C	-4.51603200	-1.77456600	-0.08482900
O	-5.21153100	-1.44537700	0.88284000
C	-4.95475800	-2.96150500	-0.95361300
C	-3.40289500	1.22938500	-0.35099500
O	-4.44964400	1.41958200	-1.01475400
O	-2.69579500	2.36215100	0.13896200
C	-3.23277400	3.61815100	-0.22525900
O	1.55884100	0.78684000	1.31590200
O	1.27783900	-1.40896200	1.24847800
C	2.37087400	-1.54232200	2.20087100
C	1.41367600	2.12843800	0.78900800
O	4.27474000	1.18998000	-0.65490000
C	5.67668500	1.55121700	-0.41743000
O	4.92359700	-0.92715000	-0.55206700
C	4.87782500	-2.30995600	-0.97416700
H	2.11784600	0.37718800	-1.77156800
H	2.42540200	-1.42272600	-1.49965900
H	-1.50625400	-0.98026700	1.40594000
H	-1.37969600	0.78068900	1.43324800
H	-0.17045900	0.69279200	-0.80605400
H	-0.24508300	-1.07547400	-0.76189800
H	-2.98104500	-1.56543800	-1.35129300
H	-2.55247600	4.36765100	0.19220700
H	-4.24239900	3.76457100	0.18642200
H	-3.28890500	3.73654700	-1.31493100
H	2.39016300	-2.60046900	2.45536700
H	2.17781000	-0.92968300	3.08269500
H	3.30595500	-1.23940400	1.72626500
H	1.93319800	2.19466400	-0.16824200
H	1.90806700	2.76515800	1.52143800
H	0.35645300	2.38857500	0.69847700
H	6.01683400	1.13932800	0.53329700
H	5.67368500	2.63923600	-0.39205000
H	6.29994200	1.18650000	-1.23511800
H	4.70087700	-2.36230600	-2.05142900
H	4.10266600	-2.85015800	-0.42250900
H	5.86138200	-2.71112500	-0.73259400
H	-5.23498700	-3.79111600	-0.29613300
H	-5.84245100	-2.66656800	-1.52864300
H	-4.18830100	-3.30949300	-1.65570200

Structure **ZW2'a anti** (Onsager/B3LYP/6-31+G*)

C	2.38175500	-0.65090100	-0.73685800
C	3.86330600	-0.34913000	-0.64532000
C	-2.69316700	-0.02617400	-0.01352200
C	-1.31423000	0.06142500	0.62618800
C	-0.09719500	-0.12770300	-0.34620300
C	1.34899300	0.09295000	0.21919400
N	-3.16001900	-1.34237600	-0.34651300
C	-4.27840500	-1.98692700	0.06290200
O	-5.11415000	-1.58361800	0.89001000
C	-4.50954500	-3.34010800	-0.62432600
C	-3.53156900	1.03636700	-0.32858100
O	-4.64457300	1.05432200	-0.92308200
O	-3.01239700	2.28925400	0.13748100
C	-3.51164900	3.42668700	-0.52493300
O	1.77490600	1.43479700	0.18390900
O	1.35515200	-0.44389200	1.52148100
C	2.56105300	-0.31927000	2.28670800
C	1.02603500	2.41699500	0.89763000
O	4.25618700	0.84057400	-0.89306200
C	5.71499900	1.17502700	-0.92676400
O	4.78751400	-1.21588500	-0.41293400
C	4.63202000	-2.66431400	-0.22871900
H	2.22942300	-1.72533600	-0.62216500
H	2.10558600	-0.37570600	-1.76153500
H	-1.22503500	-0.69234300	1.41923900
H	-1.23535700	1.03118800	1.11774400
H	-0.20586300	0.55164100	-1.20093700
H	-0.13407800	-1.14935600	-0.75112900
H	-2.60588200	-1.86084600	-1.02175700
H	-3.00796200	4.28875900	-0.07189500
H	-4.60290500	3.52789300	-0.40921800
H	-3.28660800	3.40704200	-1.60233200
H	2.29805500	-0.58588400	3.31163000
H	2.95614000	0.70036600	2.26057800
H	3.33115000	-1.01996000	1.94109900
H	0.08813600	2.65624700	0.38225700
H	1.66434100	3.30319900	0.92466900
H	0.80994400	2.09171900	1.92183800
H	6.14639400	0.96904600	0.05263400
H	5.72802500	2.23508600	-1.16415900
H	6.19215400	0.57766300	-1.70415900
H	3.95538800	-2.85948300	0.60437200
H	5.64035000	-3.00864500	-0.00165000
H	4.28126600	-3.10024400	-1.16520000
H	-4.80219700	-4.07297000	0.13579800
H	-3.63723000	-3.72468300	-1.16540000
H	-5.33863200	-3.24171500	-1.33952500

Structure **4'a** (Onsager/B3LYP/6-31+G*)

C	-0.80283300	0.15097400	-0.16123500
C	0.00463200	0.43798500	-1.45398000
C	1.25988400	1.26949300	-1.19604000
C	2.22291600	0.54858500	-0.25107000
C	1.49007300	0.14617500	1.03692200
C	0.13694600	-0.59353200	0.88233800
N	-1.23893600	1.37589700	0.50857600
O	2.75269400	-0.65781700	-0.79099000
O	3.26437400	1.48382700	0.00994900
O	-0.37324600	-0.52610800	2.22437900
O	0.21075000	-1.90782600	0.41473200
C	-2.06532100	-0.69889100	-0.48200400
O	-1.93266700	-1.43659900	-1.59369100
O	-3.07587600	-0.68753300	0.19220500
C	-3.06186300	-2.25789300	-1.94017000
C	-2.11400400	2.27495900	-0.03784000
O	-2.45749300	2.25234800	-1.21830600
C	-2.64323800	3.32694900	0.92538200
C	1.17196300	-2.78777900	1.00998500
C	-1.41237900	-1.42018800	2.65451900
C	3.44051600	-0.56545100	-2.03660800
C	4.29189900	1.08058700	0.91443800
H	-0.64825700	0.95164600	-2.16175000

H	0.27817300	-0.52580300	-1.88909800
H	1.76557600	1.49647300	-2.14042300
H	1.00317800	2.23178600	-0.74157000
H	2.13546800	-0.47029200	1.66701400
H	1.28887200	1.06450800	1.59494500
H	-1.19550700	1.32558100	1.52123700
H	-2.77533300	-2.76588900	-2.86153000
H	-3.94773000	-1.63666700	-2.09668500
H	-3.26056900	-2.98258600	-1.14595900
H	0.87252800	-3.79346100	0.70599600
H	1.15471800	-2.72130700	2.10411500
H	2.17492800	-2.57367500	0.63152100
H	-1.25255200	-1.56069900	3.72714600
H	-1.34413400	-2.38512600	2.14552100
H	-2.39965900	-0.98984700	2.47079500
H	4.00140500	-1.49756400	-2.14165300
H	4.13560400	0.28179000	-2.04935000
H	2.74083000	-0.47754400	-2.87824600
H	5.09203800	1.81691100	0.80708400
H	4.67837800	0.08487000	0.66808000
H	3.94258900	1.08824900	1.95544800
H	-3.67533800	3.06816700	1.18998400
H	-2.65984000	4.29507900	0.41739000
H	-2.05626100	3.40994100	1.84591500

Structure **4'a** (PCM/B3LYP/6-31+G*)

C	-0.80765900	0.14974200	-0.15437600
C	-0.00001000	0.43197400	-1.44911800
C	1.25525100	1.26527100	-1.19753400
C	2.22027600	0.54339000	-0.25572800
C	1.49177500	0.14983600	1.03730000
C	0.13607300	-0.58855100	0.89119500
N	-1.24505100	1.37876900	0.50660800
O	2.74457300	-0.66420800	-0.79407400
O	3.26843100	1.47744200	-0.00030200
O	-0.36588300	-0.51651000	2.23453600
O	0.20736800	-1.90577200	0.42870300
C	-2.06839900	-0.70449100	-0.47686900
O	-1.92718500	-1.44757900	-1.58147200
O	-3.08441200	-0.68908000	0.19095400
C	-3.04872600	-2.28203400	-1.93482500
C	-2.11124700	2.27965500	-0.04132700
O	-2.48506500	2.22218800	-1.21612300
C	-2.58600400	3.38113300	0.89008700
C	1.16019000	-2.78625000	1.03637300
C	-1.42438100	-1.38949500	2.66345800
C	3.41983400	-0.57887200	-2.04877600
C	4.30220400	1.06499800	0.89506600
H	-0.65263300	0.94184100	-2.15968100
H	0.27418700	-0.53250000	-1.88160100
H	1.75500200	1.49090600	-2.14544300
H	0.99840300	2.22728800	-0.74179100
H	2.13795700	-0.46605500	1.66739100
H	1.29662800	1.07158200	1.59309000
H	-1.15214900	1.37091400	1.51699700
H	-2.74968900	-2.79214800	-2.85068100
H	-3.93772600	-1.66947600	-2.10554000
H	-3.24697200	-3.00394700	-1.13825800
H	0.85616000	-3.79313400	0.74063600
H	1.13844300	-2.70979700	2.12966800
H	2.16648300	-2.58080900	0.66127000
H	-1.26810600	-1.53613700	3.73567500
H	-1.37728800	-2.35428600	2.15190800
H	-2.40108100	-0.93507700	2.48262100
H	3.96709600	-1.51828800	-2.16060300
H	4.12661500	0.25842900	-2.06801600
H	2.71284400	-0.47963300	-2.88238400
H	5.10512000	1.79831400	0.78604200
H	4.68185400	0.06941200	0.63862800
H	3.95951200	1.06763200	1.93802400
H	-3.66202900	3.25878800	1.05853200
H	-2.43517600	4.34889500	0.40171600
H	-2.07578000	3.38621800	1.85820900

Structure **5'a** (Onsager/B3LYP/6-31+G*)

C	0.00000000	0.00000000	0.00000000
C	1.54765966	0.00000000	0.00000000
C	2.11106275	1.42198867	0.00000000
C	1.58494740	2.24721814	1.16330988
C	0.24367619	1.91584652	1.65691626
C	-0.49919086	0.91723439	1.12065797
N	-0.59307064	0.51678819	-1.24098941
O	2.23598820	3.17296459	1.64435058
O	-1.77650177	0.62748857	1.43297783
C	-0.53738470	-1.44130587	0.24033385
O	-0.08238324	-1.94636264	1.39783224
O	-1.26847414	-2.02695946	-0.52475991
C	-0.56525513	-3.26439900	1.74675361
C	-0.26882089	0.10744756	-2.52026181
O	0.78290738	-0.44846431	-2.81713269
C	-1.32999080	0.42700627	-3.56110392
C	-2.44847353	1.39472021	2.44353674
H	1.90452019	-0.55938683	-0.86436094
H	1.86643761	-0.52011964	0.90874536
H	3.20469248	1.41366598	0.05082979
H	1.83456229	1.93734658	-0.93077311
H	-0.14056879	2.55087166	2.44788680
H	-1.56580055	0.78018507	-1.12691774
H	-0.11344060	-3.48860261	2.71268928
H	-0.25435749	-3.99019658	0.99152376
H	-1.65517578	-3.25592151	1.81976931
H	-3.45139265	0.97381377	2.50957016
H	-2.49892614	2.44979840	2.15343410
H	-1.93281678	1.29135472	3.40383910
H	-1.90102253	1.33225110	-3.32787326
H	-0.84942719	0.53780235	-4.53542225
H	-2.03052429	-0.41540915	-3.61551354

Structure **5'a** (PCM/B3LYP/6-31+G*)

C	0.00000000	0.00000000	0.00000000
C	1.55092851	0.00000000	0.00000000
C	2.11268620	1.42397904	0.00000000
C	1.57223388	2.25715961	1.14735388
C	0.24262003	1.91524859	1.65487405
C	-0.49433209	0.90115420	1.13701256
N	-0.55344216	0.53866573	-1.24741734
O	2.21064836	3.20183525	1.61870604
O	-1.74535616	0.57574862	1.50298093
C	-0.56464913	-1.43222915	0.23675060
O	0.01925189	-2.00576899	1.29918421
O	-1.42744768	-1.95239823	-0.43439933
C	-0.45373350	-3.32321898	1.65975757
C	-0.33443653	-0.00252036	-2.48999091
O	0.50273472	-0.87988086	-2.70202777
C	-1.20582047	0.55949944	-3.59850368
C	-2.38814943	1.31744664	2.55311103
H	1.90382781	-0.55532784	-0.86941287
H	1.88640929	-0.52657090	0.89822096
H	3.20566118	1.41279477	0.06261968
H	1.85096287	1.93931349	-0.93561666
H	-0.13859267	2.54239298	2.45390383
H	-1.35318135	1.15498608	-1.15724743
H	0.12777427	-3.60610727	2.53690464
H	-0.28013831	-4.02194354	0.83780207
H	-1.52001373	-3.28614395	1.89625458
H	-3.37053700	0.86027683	2.66975178
H	-2.49226593	2.36991556	2.26877920
H	-1.81733022	1.23013957	3.48341619
H	-1.60628135	1.55271133	-3.37070899
H	-0.62399379	0.60348493	-4.52253545
H	-2.04947584	-0.12245379	-3.76012474

Structure **2b** (B3LYP/6-31+G*)

C	-1.30314600	2.04102600	0.00045000
C	-1.10559700	0.71203400	-0.00941100
H	-0.47824100	2.74027400	-0.00241800
H	-2.31840400	2.41729100	0.01191000
N	0.13595700	0.04783000	-0.02252200
C	-2.22205800	-0.28655400	-0.00725300
C	1.36568300	0.62445800	-0.01688200
O	-3.43878500	0.26840900	0.01128800
O	-2.01703300	-1.48991800	-0.02098900
H	0.06306900	-0.96691000	-0.03701800
C	2.54246700	-0.39095200	0.00287800

C	-4.55333200	-0.64925100	0.01598300
O	1.61680600	1.81680100	-0.00997200
H	-5.44059400	-0.01705700	0.03521500
H	-4.51073900	-1.28828800	0.90124400
H	-4.53503200	-1.26794300	-0.88445900
F	2.12835900	-1.67747700	-0.14933400
F	3.19904000	-0.31378100	1.17590600
F	3.40996000	-0.12197300	-0.98479700

Structure **2b** (Onsager/B3LYP/6-31+G*)

C	-1.31339300	2.05533300	-0.00064500
C	-1.11399800	0.72816300	-0.00785100
H	-0.49073900	2.75757600	-0.00328900
H	-2.32978700	2.42937800	0.00790800
N	0.13241200	0.06535900	-0.01784100
C	-2.22256300	-0.28514800	-0.00582400
C	1.36128500	0.62895900	-0.01295000
O	-3.43647700	0.25480400	0.00880900
O	-1.98714600	-1.48457200	-0.01654800
H	0.04373300	-0.94983100	-0.02998800
C	2.52958900	-0.39596600	0.00190500
C	-4.55819600	-0.66530800	0.01311900
O	1.63738200	1.81864900	-0.00614400
H	-5.44275300	-0.03069100	0.02726400
H	-4.51587400	-1.29795100	0.90211600
H	-4.53445900	-1.28393000	-0.88635400
F	2.12026600	-1.68337400	-0.12608100
F	3.21535900	-0.30515200	1.16184100
F	3.39066100	-0.14361800	-1.00334100

Structure **2b** (PCM/B3LYP/6-31+G*)

C	-1.30914800	2.04237700	0.00033500
C	-1.10954200	0.71442500	-0.00005800
N	0.13506600	0.05281200	-0.00057400
C	1.36197100	0.62172800	-0.00129200
C	2.53770600	-0.39403200	0.00002300
C	-2.22382700	-0.28864100	0.00010500
O	-3.43612200	0.26277800	0.00010900
C	-4.56038500	-0.64841900	0.00000600
O	-2.00835100	-1.49223100	-0.00013900
O	1.62535500	1.81513700	-0.00048000
H	-0.48676900	2.74448900	0.00028900
H	-2.32461900	2.41865500	0.00072200
H	-5.44200600	-0.00855000	-0.00019700
H	-4.53363100	-1.27428500	0.89504800
H	-4.53333000	-1.27441800	-0.89493400
H	0.05909300	-0.96232200	-0.00050800
F	2.12652700	-1.68646600	-0.00153300
F	3.30645700	-0.21211700	1.09085000
F	3.31013700	-0.21067800	-1.08787600

Structure **TS0b** (B3LYP/6-31+G*)

C	-2.78812600	3.05756000	0.08438800
O	-2.11127900	1.88864700	-0.39665300
C	-0.77805100	1.80732100	-0.05825100
O	-0.25271600	2.62881100	0.70481200
C	-0.08372200	0.72332700	-0.68287800
N	1.27056800	0.65273400	-0.25309700
C	2.14362200	-0.35839500	-0.39393500
O	1.93727900	-1.46565400	-0.90260000
C	-0.64928100	-0.17071400	-1.63725600
C	-1.23599200	-1.81903000	-1.07268300
C	-2.23841000	-1.61615900	-0.09871500
O	-3.48610200	-1.43633400	-0.49750500
C	-4.46218400	-0.90068700	0.42410400
O	-2.02201900	-1.36431200	1.17746200
C	-0.74250000	-1.69032800	1.78101600
C	3.56074200	-0.06302100	0.15003700
H	-1.62496700	-2.25076200	-1.99234700
H	-0.31251800	-2.27901800	-0.73704500
H	-1.55276100	0.22129900	-2.09874500
H	0.05375100	-0.57357400	-2.36328000
H	1.56016200	1.48402500	0.25963800
H	-3.81150600	2.97468500	-0.28777700
H	-2.31760000	3.96581000	-0.30393200
H	-2.77729700	3.09463300	1.17780400
H	0.05502900	-1.10214600	1.33105800
H	-0.55038100	-2.76102900	1.66839300
H	-0.86124800	-1.42987100	2.83190700
H	-4.15620600	0.09817900	0.74325800
H	-4.57507300	-1.56021000	1.28772800
H	-5.38711300	-0.85782600	-0.14980800
F	3.66461800	1.15101000	0.75590900
F	4.47055500	-0.09329700	-0.84496700
F	3.91881200	-0.99347400	1.06080700

Structure **TS1b anti** (Onsager/B3LYP/6-31+G*)

C	-2.90086100	-1.22995700	0.41090800
C	-1.66815200	-0.71824800	0.84337900
C	-0.72097400	-0.05420700	-0.77292500
C	0.33440200	0.81492200	-0.43539200
N	1.63492200	0.38655300	-0.05909100
C	0.18356400	2.23158800	-0.22178000
O	-1.08446800	2.68991600	-0.42803800
C	-1.26864700	4.10952200	-0.29552200
C	2.24037300	-0.78691500	-0.30046700
C	3.70361900	-0.85620500	0.19899600
O	-4.02909400	-0.55171200	0.28349900
C	-4.15931400	0.77183200	0.85407900
O	-2.94511300	-2.45575500	-0.08371700
C	-4.19389100	-2.97728100	-0.61280900
O	1.10731900	2.98012000	0.12873600
O	1.77997300	-1.78933900	-0.85012700
H	-0.95462100	-1.46935900	1.16572700
H	-1.70514000	0.17353200	1.45734900
H	-1.55130900	0.43155700	-1.27423600
H	-0.46157300	-1.03032200	-1.16729200
H	2.18227400	1.14747000	0.34012600
H	-2.32166000	4.28758600	-0.51692300
H	-0.63442700	4.64652500	-1.00652200
H	-1.02933100	4.43665500	0.71997100
H	-3.42745000	1.44922000	0.40695600
H	-4.03359100	0.71931200	1.93908400
H	-5.17359200	1.08313900	0.60856800
H	-4.52616000	-2.37893900	-1.46327400
H	-4.95918300	-2.98369200	0.16589000
H	-3.95349800	-3.99245900	-0.92426700
F	4.15513700	0.29491500	0.77757400
F	3.86943600	-1.84097400	1.11108500
F	4.55044600	-1.12530100	-0.82767500

Structure **TS1b anti** (PCM/B3LYP/6-31+G*)

C	-2.78513100	-1.28514000	0.43259200
C	-1.57777800	-0.70539200	0.84386900
C	-0.74345200	0.00813100	-0.78653500
C	0.31111400	0.88652100	-0.46424500
N	1.60829500	0.44842500	-0.09155500
C	0.14185900	2.29430200	-0.22312600
O	-1.13190200	2.74178000	-0.43075100
C	-1.33538200	4.15534400	-0.26795500
C	2.19161000	-0.73444500	-0.33795400
C	3.63386000	-0.86043800	0.20589500
O	-3.94982700	-0.66474500	0.31383300
C	-4.11022700	0.66833100	0.85229600
O	-2.76684400	-2.51310000	-0.06321700
C	-3.97021800	-3.07869400	-0.63980200
O	1.05155200	3.05087400	0.14786000
O	1.70903300	-1.71107100	-0.92000500
H	-0.81398000	-1.41620800	1.14350200
H	-1.65005300	0.17433100	1.47275500
H	-1.59679300	0.49128300	-1.25151500
H	-0.48092200	-0.95176500	-1.21643600
H	2.16556200	1.18484600	0.33701400
H	-2.38903700	4.32385200	-0.49539600
H	-0.70301800	4.71802800	-0.96060300
H	-1.11239100	4.46273500	0.75760200
H	-3.40583500	1.35591500	0.37766500
H	-3.96454200	0.64994000	1.93618100
H	-5.13617400	0.94532700	0.61281700
H	-4.30179100	-2.47979800	-1.49085100
H	-4.75818300	-3.13517900	0.11472000
H	-3.67501200	-4.07615300	-0.96298600
F	4.10689900	0.28128600	0.77351200
F	3.70854200	-1.83148000	1.14487400

F	4.48794500	-1.19504400	-0.78566900

Structure **TS1b gauche** (Onsager/B3LYP/6-31+G*)

C	-2.37471900	3.16421800	-0.15951700
O	-1.74282500	1.94813000	-0.59306100
C	-0.44965400	1.77502300	-0.20033200
O	0.14505400	2.60132500	0.50800100
C	0.14531000	0.55389800	-0.67456000
N	1.45791800	0.39526600	-0.15219800
C	2.41656200	-0.46611500	-0.52675800
O	2.35167700	-1.36770800	-1.36808100
C	-0.52977900	-0.44655600	-1.40779800
C	-1.40072200	-1.86456300	-0.38763500
C	-2.64262200	-1.40751900	0.09168500
O	-3.67279300	-1.41600000	-0.72825800
C	-4.96087200	-0.89640700	-0.29751700
O	-2.87198100	-0.83633100	1.26218800
C	-1.88186600	-0.89824000	2.31218800
C	3.76118800	-0.28032200	0.21367200
H	-1.49844900	-2.59953200	-1.18104400
H	-0.65006100	-2.11409200	0.35431600
H	-1.39349700	-0.09829900	-1.96576900
H	0.10295100	-1.13920100	-1.95247200
H	1.69709400	1.14321600	0.49806200
H	-3.37858000	3.13617200	-0.58484000
H	-1.82751500	4.03580500	-0.52942600
H	-2.42267600	3.20738400	0.93208900
H	-0.97175700	-0.37631500	2.01159500
H	-1.67330100	-1.94288600	2.56136000
H	-2.34368700	-0.39462600	3.16057100
H	-4.87618800	0.16690500	-0.06621400
H	-5.31623900	-1.45047100	0.57334100
H	-5.61808500	-1.05811100	-1.14996100
F	3.76076300	0.72507300	1.13282600
F	4.75734600	0.00326000	-0.66667600
F	4.12573000	-1.40818200	0.86461600

Structure **TS1b gauche** (PCM/B3LYP/6-31+G*)

C	-2.69283300	3.05392200	0.03528600
O	-1.99125600	1.91872900	-0.49639100
C	-0.69489000	1.77662500	-0.09304000
O	-0.17469400	2.54536400	0.73172500
C	-0.00413900	0.68009700	-0.71403500
N	1.30489500	0.53176000	-0.17987200
C	2.29334100	-0.28235500	-0.58093600
O	2.26646700	-1.12102500	-1.48805400
C	-0.58668600	-0.23227500	-1.62126700
C	-1.30743900	-1.89857900	-0.89798800
C	-2.36860500	-1.55783400	-0.04839500
O	-3.56881100	-1.36911800	-0.56958600
C	-4.63155100	-0.82158900	0.24751100
O	-2.26147700	-1.23069500	1.22707300
C	-1.06104500	-1.56624400	1.96486700
C	3.60639000	-0.13485100	0.22270700
H	-1.61556300	-2.37317200	-1.82573500
H	-0.42816200	-2.33918800	-0.44148800
H	-1.48635800	0.13086900	-2.10858000
H	0.09404900	-0.76491700	-2.27616200
H	1.50583500	1.22189700	0.54227800
H	-3.68815500	3.01270900	-0.40990300
H	-2.19122800	3.98459200	-0.24555600
H	-2.75830400	2.99447300	1.12553200
H	-0.19908100	-1.04099400	1.55144600
H	-0.90858000	-2.64909100	1.94311100
H	-1.25666100	-1.23027200	2.98248300
H	-4.36161700	0.18048400	0.58722200
H	-4.82740400	-1.47369700	1.10155800
H	-5.49540300	-0.78477300	-0.41502500
F	3.55434600	0.82343400	1.18636800
F	4.63226100	0.18098100	-0.59753100
F	3.92509200	-1.29761100	0.83577700

Structure **ZW1'b** (B3LYP/6-31+G*)

C	-2.84525200	2.94963600	0.04103100
O	-2.15151200	1.76896400	-0.37568600
C	-0.79447300	1.74513600	-0.05047100
O	-0.30231300	2.61893000	0.68381700
C	-0.09337900	0.66627000	-0.63256400
N	1.29131500	0.66580600	-0.30147000
C	2.10736200	-0.39194900	-0.22303900
O	1.80331100	-1.58461600	-0.39549900
C	-0.64581900	-0.25625900	-1.62621300
C	-1.18625600	-1.73829100	-1.12003100
C	-2.20352600	-1.54530400	-0.10865900
O	-3.44737500	-1.45972500	-0.51179000
C	-4.46684700	-0.96915800	0.39679900
O	-2.00179800	-1.26550600	1.14234000
C	-0.71309800	-1.39508800	1.82690700
C	3.57999100	-0.05916900	0.09168700
H	-1.62507500	-2.23595900	-1.98664500
H	-0.30342500	-2.26836200	-0.76732800
H	-1.49994800	0.19706300	-2.13386200
H	0.09946200	-0.55033800	-2.37103000
H	1.63816000	1.57101800	0.00936500
H	-3.87489100	2.82254800	-0.30313000
H	-2.40685800	3.84288400	-0.41522100
H	-2.81549300	3.06346700	1.12916900
H	0.08079400	-1.68386500	1.14087000
H	-0.87135100	-2.14601800	2.60412100
H	-0.50666500	-0.41843000	2.26195100
H	-4.20975900	0.04558700	0.70637000
H	-4.54893900	-1.62973300	1.26243400
H	-5.38371900	-0.98193900	-0.19020300
F	3.78428000	1.25581600	0.37613100
F	4.38057300	-0.37093600	-0.95124400
F	4.00778900	-0.76797800	1.15792400

Structure **ZW1'b anti** (Onsager/B3LYP/6-31+G*)

C	-2.95592200	-1.16131200	0.33859200
C	-1.67744000	-0.52252100	0.69662400
C	-0.80793500	-0.14423400	-0.62396700
C	0.32006900	0.77032400	-0.33168200
N	1.63163500	0.33627200	-0.01321500
C	0.18612900	2.16008000	-0.13194000
O	-1.10986500	2.62099300	-0.28908800
C	-1.28597200	4.03779700	-0.18038300
C	2.27251500	-0.80462500	-0.29315100
C	3.74874100	-0.81624100	0.14748100
O	-4.06567500	-0.54216100	0.08914500
C	-4.26391600	0.88660700	0.35256300
O	-2.96053700	-2.44002200	0.13507900
C	-4.19763500	-3.12565700	-0.27952600
O	1.11737900	2.94160700	0.17543800
O	1.84090400	-1.83014000	-0.84440200
H	-1.09104900	-1.21788300	1.29975900
H	-1.85734400	0.39553000	1.25631400
H	-1.49095200	0.33744800	-1.32925500
H	-0.46458600	-1.08631400	-1.05521900
H	2.17182200	1.11138400	0.37225100
H	-2.35058400	4.21699000	-0.34187100
H	-0.69863000	4.56220600	-0.94122500
H	-0.98810700	4.39492200	0.80989700
H	-3.44671900	1.46379100	-0.08134000
H	-4.33605500	1.02976200	1.43237700
H	-5.21541800	1.11502100	-0.12384600
H	-4.52408700	-2.73347900	-1.24309700
H	-4.96439200	-2.97615600	0.48159600
H	-3.90915300	-4.17147900	-0.35020000
F	4.18934800	0.33844900	0.74069900
F	4.58187200	-1.01865600	-0.91864600
F	4.02148700	-1.81747700	1.02342900

Structure **ZW1'b anti** (PCM/B3LYP/6-31+G*)

C	-2.68864400	-1.30740700	0.37980600
C	-1.43173100	-0.63393900	0.66818300
C	-0.81800200	-0.02830600	-0.73469400
C	0.27830500	0.91871800	-0.48750900
N	1.56957800	0.47514800	-0.10119700
C	0.08718500	2.29338200	-0.22219400
O	-1.22052200	2.71922400	-0.39202200
C	-1.44079200	4.12613600	-0.23659500
C	2.17277800	-0.68950400	-0.37081100
C	3.59237000	-0.82514500	0.21533700
O	-3.86054300	-0.73707400	0.34353000

C	-4.04767100	0.63431700	0.80902900
O	-2.63958500	-2.53497000	-0.05041100
C	-3.85131100	-3.20375900	-0.51538500
O	0.97823000	3.08966200	0.14568100
O	1.71690000	-1.65436100	-1.00539500
H	-0.70448900	-1.34641100	1.06057000
H	-1.56878300	0.18838900	1.36938800
H	-1.62841800	0.48095700	-1.25931100
H	-0.50665100	-0.90272900	-1.30697500
H	2.11080900	1.20470500	0.35993600
H	-2.50559100	4.27820500	-0.42509100
H	-0.84737100	4.69696400	-0.95788300
H	-1.18556700	4.45504500	0.77532800
H	-3.36074300	1.30364100	0.28834900
H	-3.89425100	0.66676900	1.89005700
H	-5.08259700	0.86342400	0.56121700
H	-4.26721800	-2.65946100	-1.36503200
H	-4.57245400	-3.25869200	0.30201700
H	-3.51400200	-4.19557100	-0.81003700
F	4.04446300	0.29981500	0.83480200
F	4.48645600	-1.12523600	-0.75521900
F	3.65014000	-1.82658800	1.12750500

Structure **ZW1'b gauche** (Onsager/B3LYP/6-31+G*)

C	-2.55188800	-1.35404900	-0.06038200
C	-1.30445400	-1.70121800	-0.76323300
C	-0.59820600	-0.40916100	-1.40255300
C	0.05254100	0.55794700	-0.48472000
N	1.44852000	0.50728500	-0.22245600
C	-0.51277100	1.77808100	-0.06432400
O	-1.86763800	1.88159700	-0.34134400
C	-2.47975000	3.12803000	0.01172700
C	2.26356900	-0.55190300	-0.20576300
C	3.73857500	-0.21259200	0.07326100
O	-2.67461900	-1.09672400	1.20230400
C	-1.55322500	-1.22740900	2.13388100
O	-3.61957600	-1.24608700	-0.77614200
C	-4.89698300	-0.83675500	-0.17796700
O	0.10377100	2.70266800	0.50924400
O	1.97867100	-1.74349000	-0.42255400
H	-1.57395000	-2.37136800	-1.58423700
H	-0.58459400	-2.19668100	-0.11144700
H	-1.36040500	0.09529200	-2.00426900
H	0.13510900	-0.84691600	-2.08559200
H	1.79933800	1.40959600	0.09855500
H	-3.52588400	3.03707800	-0.28681600
H	-2.00877400	3.95952700	-0.52180100
H	-2.40620200	3.31068700	1.08800300
H	-0.70726900	-0.64869300	1.76555800
H	-1.31454800	-2.28740700	2.24540700
H	-1.93828900	-0.82007100	3.06685900
H	-4.78264400	0.15753500	0.25455200
H	-5.19059000	-1.56598900	0.57807100
H	-5.59381000	-0.83379800	-1.01281200
F	3.96219200	1.08655600	0.43913100
F	4.52355800	-0.43322700	-1.02179400
F	4.24797700	-0.98214100	1.06439000

Structure **ZW1'b gauche** (PCM/B3LYP/6-31+G*)

C	-2.34862500	-1.44478800	-0.11679600
C	-1.21910100	-1.68488700	-1.02156000
C	-0.62626300	-0.28902300	-1.55174900
C	-0.03699000	0.64136200	-0.55765100
N	1.35152800	0.60785800	-0.24699600
C	-0.68061200	1.77074200	-0.02913600
O	-2.03516700	1.83858300	-0.34496500
C	-2.71504600	3.01830300	0.09299200
C	2.17979900	-0.44082600	-0.24951000
C	3.64272400	-0.10509100	0.09446100
O	-2.28065900	-1.31142000	1.16641400
C	-1.04891500	-1.58345800	1.91670200
O	-3.51106100	-1.25574900	-0.65315100
C	-4.64883900	-0.86048400	0.17342800
O	-0.14197600	2.66595800	0.66469300
O	1.90681400	-1.62428900	-0.52461100
H	-1.58659700	-2.24421200	-1.88687300
H	-0.41099200	-2.23211900	-0.53645300
H	-1.43935000	0.20796200	-2.08833700
H	0.11911800	-0.60459000	-2.28840100
H	1.69474800	1.49659200	0.11298400
H	-3.74581100	2.90828100	-0.25183100
H	-2.27017900	3.91699300	-0.34668700
H	-2.68964000	3.10783800	1.18376700
H	-0.25022300	-0.94852400	1.54063100
H	-0.81092600	-2.64493500	1.82266500
H	-1.30740600	-1.33186600	2.94361700
H	-4.42343400	0.09254500	0.65351900
H	-4.84765300	-1.63634000	0.91458600
H	-5.47281300	-0.76620000	-0.53098600
F	3.82882000	1.17448500	0.52170500
F	4.45234500	-0.28072100	-0.98063900
F	4.10639800	-0.91734100	1.07145000

Structure **TS2b** (Onsager/B3LYP/6-31+G*)

C	3.03410200	3.05323000	-0.14231900
O	2.32399000	1.92903000	0.38819400
C	1.03590300	1.77027700	-0.06155900
O	0.53621000	2.56831900	-0.87890900
C	0.35963900	0.63220400	0.47445200
C	1.86243600	-1.54042300	0.19719100
O	3.02538200	-0.97292800	0.17266400
C	3.80921200	-0.93746200	-1.05397000
C	1.14567600	-1.51488300	1.51870200
C	0.77554000	-0.04041400	1.77273200
O	1.55717900	-2.26385000	-0.83975500
C	0.35039600	-3.08313200	-0.89349000
N	-1.02093000	0.70861200	0.12397100
C	-1.98042700	-0.20521800	0.27662900
O	-1.87554600	-1.34829900	0.75729500
H	1.81200400	-1.94000800	2.28453900
H	0.23876900	-2.11510800	1.45865000
H	1.64663700	0.49010400	2.16691300
H	-0.01291600	0.00684000	2.53603800
H	-1.22535700	1.55468100	-0.41194000
H	4.02465300	3.01320900	0.31466600
H	2.53303900	3.99080600	0.11867600
H	3.11305500	2.98880800	-1.23205000
H	0.27555700	-3.37789800	-1.93889100
H	-0.51778200	-2.50541700	-0.56919100
H	0.49830600	-3.96128300	-0.26164800
H	3.23532300	-0.42670900	-1.82950400
H	4.06145100	-1.95403200	-1.35970700
H	4.70161100	-0.37502500	-0.78882200
C	-3.37671100	0.23783900	-0.19986800
F	-3.39615800	1.45808300	-0.80929600
F	-4.25086200	0.31270000	0.83839800
F	-3.89410800	-0.64628600	-1.08270600

Structure **TS2b** (PCM/B3LYP/6-31+G*)

C	3.17868800	2.91391700	-0.10599500
O	2.40908100	1.84315000	0.45432400
C	1.13759900	1.69507400	-0.04187900
O	0.69777700	2.46661900	-0.92170800
C	0.40558500	0.60665400	0.51612900
C	1.75717000	-1.55678000	0.17587300
O	2.95300700	-1.05220200	0.10697400
C	3.64305500	-0.98638400	-1.17073200
C	1.12340900	-1.55301300	1.54189900
C	0.78359000	-0.07568700	1.82194900
O	1.37001100	-2.23657200	-0.86425200
C	0.13842800	-3.01959600	-0.87725000
N	-0.96277200	0.71084200	0.12828500
C	-1.97221300	-0.13415000	0.34024000
O	-1.93342800	-1.23653500	0.91734300
H	1.82882600	-1.99477400	2.26122000
H	0.21200500	-2.14960700	1.52594700
H	1.66185000	0.43119000	2.23049500
H	-0.01290700	-0.01154900	2.57339800
H	-1.13056400	1.53268800	-0.45381700
H	4.14467600	2.87298000	0.40089300
H	2.69719000	3.87962300	0.07572000
H	3.31058700	2.78022400	-1.18439700
H	-0.01537100	-3.25975000	-1.92817700
H	-0.69010700	-2.43719500	-0.47064600

H	0.30167500	-3.93004900	-0.29652800
H	3.03551400	-0.42023800	-1.87992100
H	3.83079900	-1.99555800	-1.54179000
H	4.57492100	-0.46871100	-0.95173800
C	-3.33174500	0.32904700	-0.21757800
F	-3.28176600	1.51931600	-0.87402900
F	-4.24337800	0.46236700	0.77503500
F	-3.82626200	-0.58116500	-1.08945300

Structure **3'b** (B3LYP/6-31+G*)

C	-4.13658500	-0.89358000	0.13266800
O	-2.90136400	-0.17257000	0.11471600
C	-1.75167000	-0.92609700	-0.13348700
O	-1.41974400	-1.78208900	0.93072100
C	-1.49091000	-1.20660200	2.24836600
C	-0.60968800	0.07466400	-0.62740800
C	-0.83022700	1.56510600	-0.35389500
O	-1.38519900	2.31866300	-1.12047000
C	-1.68250500	-1.62984300	-1.50862200
C	-0.91880100	-0.40328900	-2.07352400
N	0.66495400	-0.40976500	-0.12191300
C	1.84237500	0.14454300	-0.47932900
O	1.99073100	1.09479300	-1.23012400
C	3.09468900	-0.52659500	0.14767200
O	-0.36726000	1.92348800	0.85974200
C	-0.51865000	3.31696100	1.19773500
H	-4.43951400	-1.18778400	-0.87914600
H	-4.87743500	-0.20268600	0.53977800
H	-2.63807200	-1.88349600	-1.97367700
H	-4.07232900	-1.78482200	0.76756500
H	-1.57000200	0.31317300	-2.57694000
H	-1.06653200	-2.53123400	-1.44873500
H	-0.04050900	-0.59950300	-2.69135900
H	-2.52868200	-1.02234600	2.54254600
H	-1.57694000	3.59034600	1.20618400
H	-1.04673800	-1.94856800	2.91509600
H	-0.93134000	-0.26674700	2.30449700
H	0.01442100	3.93658600	0.47250300
H	0.64104700	-1.19929100	0.51488200
H	-0.08155900	3.42199600	2.19097500
F	3.87336800	-1.05510600	-0.81461800
F	3.82091100	0.37456700	0.83007100
F	2.77616900	-1.53247900	1.01026800

Structure **3'b** (Onsager/B3LYP/6-31+G*)

C	-4.11943600	-0.93144700	0.10853800
O	-2.88566000	-0.19841900	0.10141300
C	-1.73040500	-0.93739900	-0.14371100
C	-0.59828500	0.08012000	-0.63914500
N	0.67941700	-0.38395900	-0.11888300
C	1.85623000	0.16105100	-0.47913800
C	3.10531400	-0.49726200	0.16746400
C	-1.64663600	-1.64194700	-1.51848100
C	-0.89094700	-0.41039400	-2.08326400
O	-1.37861800	-1.78775200	0.91659700
C	-1.51245600	-1.24456100	2.24525100
C	-0.84352800	1.56532900	-0.36747500
O	-0.44230900	1.91422200	0.87072900
C	-0.67856500	3.28654200	1.24150000
O	-1.36621500	2.32391500	-1.15238800
O	2.01942900	1.09541900	-1.25032400
H	-4.42918400	-1.18973200	-0.91039900
H	-4.85974900	-0.26155200	0.54887900
H	-2.59842600	-1.90395900	-1.98601600
H	-4.04060900	-1.84319600	0.71025000
H	-1.54530400	0.29692700	-2.59570100
H	-1.02465700	-2.53876700	-1.45329000
H	-0.00610200	-0.60103200	-2.69421800
H	-2.56397500	-1.10300600	2.50913600
H	-1.74787800	3.50880400	1.20112200
H	-1.06638600	-1.98828600	2.90808900
H	-0.98667700	-0.28834200	2.33959700
H	-0.13934400	3.95545900	0.56567100
H	0.64723500	-1.15966100	0.53655200
H	-0.30233200	3.37905000	2.26058000
F	2.79506300	-1.48340500	1.04810600
F	3.83462100	0.42155600	0.82823600
F	3.89106400	-1.04195900	-0.78584400

Structure **3'b** (PCM/B3LYP/6-31+G*)

C	-4.13431800	-0.88980800	0.16201900
O	-2.89699600	-0.16578600	0.10870700
C	-1.75238400	-0.92581500	-0.13763200
O	-1.40943400	-1.77197700	0.92864300
C	-1.48113900	-1.19480200	2.24900000
C	-0.60973400	0.07164200	-0.64649400
C	-0.82170200	1.56218300	-0.37165500
O	-1.34955700	2.32803700	-1.15078100
C	-1.69050000	-1.63911100	-1.50863300
C	-0.92392900	-0.42083400	-2.08661400
N	0.66663900	-0.41223700	-0.14029900
C	1.84363200	0.13163700	-0.49503400
O	2.00444800	1.08440700	-1.24683200
C	3.09061100	-0.52379000	0.15779900
O	-0.38522400	1.90818900	0.84968700
C	-0.55778700	3.29223500	1.22345000
H	-4.42653700	-1.24838000	-0.83145100
H	-4.87857000	-0.17636300	0.52047900
H	-2.64867400	-1.88973000	-1.96930000
H	-4.07211900	-1.73730000	0.85323000
H	-1.57570700	0.28917100	-2.59855900
H	-1.07688400	-2.54229200	-1.44869400
H	-0.04852400	-0.63035300	-2.70485200
H	-2.51865300	-1.01027400	2.54141100
H	-1.61935800	3.55194500	1.22202900
H	-1.03771900	-1.93713300	2.91539900
H	-0.91981600	-0.25639800	2.30350600
H	-0.01729200	3.93813700	0.52706700
H	0.63714700	-1.22070400	0.47432400
H	-0.14113800	3.37308100	2.22726200
F	3.99216200	-0.85778600	-0.78432300
F	3.67918900	0.34212900	1.00849100
F	2.79475800	-1.64678100	0.86001100

Structure **TS3b** (Onsager/B3LYP/6-31+G*)

C	3.24302900	-0.32258600	-1.29527400
C	4.55760300	-0.26087900	-0.85477800
C	-2.01416100	0.78006800	0.18481400
C	-0.84752300	0.06979600	0.81152600
C	0.41490600	-0.04437400	-0.13935300
C	1.63146100	-0.50158400	0.61935300
N	-3.23342900	0.15205900	-0.17579100
C	-3.83505900	-0.96591200	0.24540500
O	-3.42921000	-1.84278900	1.03128800
C	-5.24048000	-1.17167500	-0.34459900
C	-2.04820900	2.14089100	-0.16104400
O	-3.01866500	2.73916600	-0.69995900
O	-0.87914400	2.82439100	0.14132100
C	-0.83797900	4.19808100	-0.24628700
O	2.24920200	0.24895000	1.50114200
O	1.69392500	-1.79149300	0.85074300
C	2.75037100	-2.31140900	1.70673800
C	2.31286100	1.69414500	1.35431300
O	5.01790300	0.87045300	-0.34244700
C	6.44859000	1.01040700	-0.04168800
O	5.43324600	-1.25450500	-0.81678600
C	5.23689200	-2.45866000	-1.58936600
H	2.79806700	0.61876200	-1.59526300
H	2.90733300	-1.21032500	-1.81716800
H	-1.14585300	-0.93426400	1.12235800
H	-0.52987600	0.60176600	1.71831600
H	0.60540800	0.92893300	-0.59127500
H	0.21827800	-0.76489600	-0.93616800
H	-3.78176300	0.79630200	-0.74761300
H	0.14516700	4.56274800	0.05864000
H	-1.62397700	4.77308000	0.25588000
H	-0.95702300	4.30576400	-1.32928000
H	2.63163400	-3.39265900	1.66770200
H	2.62757800	-1.93906500	2.72475400
H	3.72106100	-2.01023200	1.30795400
H	2.94464200	1.92837500	0.49649000
H	2.79012400	2.03835800	2.27073900
H	1.31016400	2.11216700	1.25066900
H	6.73325700	0.32556200	0.75763800

H	6.55683000	2.04598100	0.27453400
H	7.03773100	0.81781800	-0.93930300
H	5.06463100	-2.20244500	-2.63795400
H	4.40049200	-3.03789900	-1.18600900
H	6.16686800	-3.01623200	-1.48425600
F	-6.20044300	-1.19644900	0.64207700
F	-5.37322900	-2.35943700	-0.99576200
F	-5.66617600	-0.21114000	-1.22762800

Structure **ZW2'b anti** (Onsager/B3LYP/6-31+G*)

C	3.02899800	-1.07965400	-1.04770600
C	4.11622500	-0.04503100	-1.04066700
C	-1.72354900	0.60332100	0.22228400
C	-0.60183600	-0.37301600	0.51979300
C	0.69330200	-0.15109200	-0.32817200
C	1.97419300	-0.90981300	0.13263400
N	-3.04813600	0.23243600	-0.11039600
C	-3.72620700	-0.91856200	-0.18734900
O	-3.34966300	-2.10182900	-0.02970800
C	-5.21167900	-0.72626600	-0.51188100
C	-1.67675200	1.99779100	0.41533400
O	-2.64496400	2.79345700	0.24066800
O	-0.45351300	2.46978600	0.84856300
C	-0.32126800	3.88712300	0.95322600
O	2.76124900	-0.23461400	1.10599400
O	1.53311700	-2.16969000	0.57945400
C	2.47492400	-3.05875000	1.18937500
C	2.15031600	0.21552400	2.32085800
O	3.83047400	1.10346900	-1.55025100
C	4.87250000	2.15358600	-1.62477700
O	5.31617700	-0.20030600	-0.62611600
C	5.89512500	-1.43361800	-0.05964800
H	3.49142100	-2.06456900	-0.97414500
H	2.51981000	-1.01771500	-2.01176700
H	-0.96141300	-1.38911100	0.34674800
H	-0.34581800	-0.32710900	1.58542700
H	0.94308900	0.91284700	-0.36875800
H	0.47120700	-0.46515700	-1.35484700
H	-3.58344300	1.09670800	-0.23396100
H	0.70080300	4.06321300	1.29442800
H	-1.03500400	4.29871600	1.67543400
H	-0.48018200	4.37053700	-0.01674200
H	1.87666800	-3.84584000	1.65224500
H	3.07181800	-2.55456500	1.95473000
H	3.13998900	-3.52333600	0.45036200
H	1.43486200	1.02026200	2.12486500
H	2.97117500	0.59091800	2.93534400
H	1.65401900	-0.61051400	2.84317500
H	5.20262300	2.39955700	-0.61539900
H	4.36744400	2.98941300	-2.10180100
H	5.70367400	1.78929800	-2.22958000
H	5.90682900	-2.20229500	-0.83346500
H	5.31829900	-1.71859100	0.81887000
H	6.91106200	-1.14723200	0.20715800
F	-6.03322700	-1.20405400	0.49500300
F	-5.61368300	-1.42048000	-1.62429700
F	-5.63650600	0.56409700	-0.72006200

Structure **4'b** (Onsager/B3LYP/6-31+G*)

C	0.23447400	0.56170600	-0.27159800
C	-0.48597300	0.10085700	-1.56369500
C	-1.16844300	-1.25829100	-1.41584000
C	-2.23399400	-1.23159200	-0.31674400
C	-1.61910700	-0.72231700	0.99626300
C	-0.80436100	0.59319600	0.93330700
N	1.28113100	-0.37557300	0.15249600
O	-3.31957200	-0.35981600	-0.60113000
O	-2.67816100	-2.57793000	-0.19586300
O	-0.13901300	0.57869700	2.20811300
O	-1.53748100	1.75972100	0.73093200
C	0.90223000	1.95116400	-0.47819400
O	0.26884200	2.69756200	-1.38834100
O	1.90354800	2.30826200	0.10949000
C	0.81037600	4.01339400	-1.61809500
C	2.35516100	-0.69925500	-0.59532400
O	2.56961800	-0.40451000	-1.76121300
C	3.39515900	-1.59786300	0.13395600
F	3.13812400	-1.75507900	1.45995000
F	4.63114900	-1.07785400	0.02312600
F	3.41520800	-2.83117400	-0.41761300
C	-2.72411000	1.96504900	1.51218700
C	0.39535600	1.79312800	2.76290300
C	-4.03996300	-0.58597900	-1.81311900
C	-3.66795800	-2.85149000	0.79676600
H	0.23848000	0.07388900	-2.38047100
H	-1.22705800	0.86549500	-1.80560000
H	-1.62302600	-1.55584800	-2.36629300
H	-0.44428900	-2.03984000	-1.16203600
H	-2.39356400	-0.59591700	1.75605100
H	-0.94444500	-1.50112200	1.36256800
H	1.33013100	-0.52164600	1.15765100
H	0.16932700	4.45680000	-2.37990900
H	1.84272100	3.93982100	-1.96969300
H	0.77800000	4.60025000	-0.69665000
H	-2.97213700	3.02124700	1.38890400
H	-2.54555000	1.75599600	2.57314600
H	-3.54242200	1.34842500	1.13282200
H	0.30961600	1.68447000	3.84738400
H	-0.17665000	2.66496000	2.43643900
H	1.44206800	1.92393700	2.47738100
H	-4.97320500	-0.02629300	-1.71734400
H	-4.26413900	-1.64917900	-1.95346000
H	-3.48957500	-0.20870500	-2.68481100
H	-4.03537800	-3.85796400	0.58355400
H	-4.50091400	-2.14160900	0.74268700
H	-3.24155700	-2.83732400	1.80849500

Structure **4'b** (PCM/B3LYP/6-31+G*)

C	0.23445000	0.56427300	-0.26670100
C	-0.48426800	0.10605200	-1.56120800
C	-1.16679500	-1.25351000	-1.41830700
C	-2.23401800	-1.22839100	-0.32128600
C	-1.62136100	-0.72504900	0.99484300
C	-0.80598100	0.59092700	0.93671100
N	1.27920500	-0.37596000	0.15518600
O	-3.31952800	-0.35585800	-0.60604500
O	-2.68283500	-2.57579100	-0.20508400
O	-0.14620200	0.57548300	2.21247200
O	-1.54144400	1.75764300	0.73501800
C	0.90611900	1.95287400	-0.47486500
O	0.26654000	2.70548000	-1.37227100
O	1.91926300	2.29989600	0.10077900
C	0.81615700	4.01885800	-1.61590800
C	2.35628500	-0.69304200	-0.58694100
O	2.58159800	-0.37450500	-1.74675300
C	3.38649600	-1.60897300	0.13284200
F	3.12564200	-1.77543500	1.45465300
F	4.62551100	-1.09593100	0.02522200
F	3.39385000	-2.83405600	-0.43477600
C	-2.71742000	1.96424800	1.53011800
C	0.40875500	1.78607500	2.75859900
C	-4.02980100	-0.57519800	-1.82562500
C	-3.67111900	-2.84842400	0.79094900
H	0.24006600	0.08005500	-2.37805400
H	-1.22452500	0.87101800	-1.80400500
H	-1.61669300	-1.54763900	-2.37210900
H	-0.44222900	-2.03464100	-1.16374400
H	-2.39696700	-0.59960000	1.75385300
H	-0.94988100	-1.50686600	1.36189700
H	1.31345200	-0.55082800	1.15648700
H	0.16544100	4.46498900	-2.36769900
H	1.84001100	3.93531500	-1.98876800
H	0.80470800	4.60756400	-0.69527400
H	-2.96202700	3.02260600	1.41595100
H	-2.52876300	1.74865300	2.58794200
H	-3.54257200	1.35208800	1.15724300
H	0.30897700	1.69477600	3.84332100
H	-0.13923500	2.66581900	2.41296100
H	1.46181800	1.88687800	2.48527200
H	-4.96035800	-0.00917700	-1.73712100
H	-4.26102500	-1.63648700	-1.96958700
H	-3.46909200	-0.20196100	-2.69209700
H	-4.03831800	-3.85586700	0.58100000
H	-4.50412000	-2.13859100	0.73496800

H	-3.24227100	-2.83069000	1.80113300

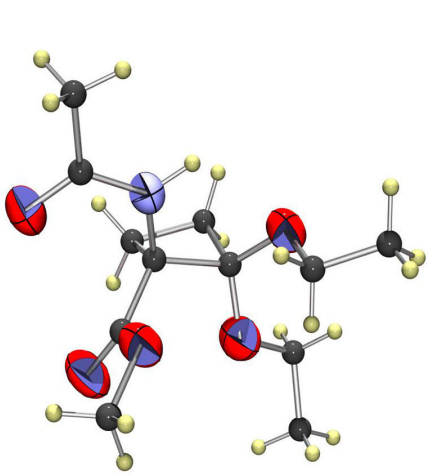
Structure **5'b** (Onsager/B3LYP/6-31+G*)

C	0.00000000	0.00000000	0.00000000
C	1.54682612	0.00000000	0.00000000
C	2.11890749	1.41879761	0.00000000
C	1.56309050	2.27239730	1.13092468
C	0.22817207	1.92769277	1.63700937
C	-0.50709134	0.91732046	1.11567683
N	-0.59114544	0.51809075	-1.24712520
O	2.18543000	3.23377881	1.57260186
O	-1.78162002	0.61655636	1.42747385
C	-0.53590322	-1.44521327	0.22079161
O	-0.11523878	-1.93585139	1.39178983
O	-1.22678892	-2.03620518	-0.57681644
C	-0.57995172	-3.26449487	1.73485438
C	-0.20538262	0.20271017	-2.50800328
O	0.80063102	-0.38219234	-2.86977522
C	-1.15739257	0.76033801	-3.60922951
F	-2.33548148	1.22613697	-3.11692981
F	-1.43796960	-0.18588039	-4.51537865
F	-0.55963144	1.79046430	-4.25267224
C	-2.45358166	1.37115151	2.44988190
H	1.91072249	-0.56820932	-0.85643973
H	1.85798061	-0.52006254	0.91087267
H	3.20953462	1.39918473	0.09203082
H	1.89044468	1.92812750	-0.94716378
H	-0.15881850	2.56802888	2.42229824
H	-1.54293518	0.85514891	-1.15055173
H	-0.15395326	-3.47084190	2.71586240
H	-0.22708308	-3.98606140	0.99457715
H	-1.67137516	-3.27767522	1.77281337
H	-3.45131723	0.93927922	2.52073230
H	-2.51625012	2.42717186	2.16631471
H	-1.92866925	1.26577908	3.40458528

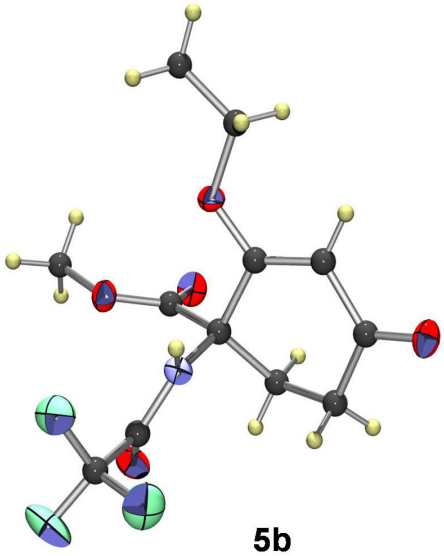
Structure **5'b** (PCM/B3LYP/6-31+G*)

C	0.00000000	0.00000000	0.00000000
C	1.54897427	0.00000000	0.00000000
C	2.12320831	1.41946009	0.00000000
C	1.58392709	2.25498370	1.14697889
C	0.22807992	1.95249765	1.61290974
C	-0.51607822	0.95370681	1.08062145
N	-0.56868310	0.46963021	-1.27512775
O	2.23686046	3.17502454	1.64179145
O	-1.79998206	0.68256233	1.37136621
C	-0.55617176	-1.42624350	0.29139363
O	-0.06178482	-1.89857717	1.43971107
O	-1.33117444	-2.01654609	-0.42740739
C	-0.52249732	-3.20746814	1.85250017
C	-0.29313237	-0.06882673	-2.48574162
O	0.56597366	-0.89052055	-2.76133976
C	-1.16168414	0.49733327	-3.64743867
F	-2.16698745	1.30375325	-3.22056834
F	-1.71631500	-0.50869645	-4.34553525
F	-0.39417999	1.21739773	-4.49059675
C	-2.48842127	1.48828596	2.34468281
H	1.91053596	-0.56648172	-0.85960606
H	1.87464060	-0.52376327	0.90371885
H	3.21536512	1.39403212	0.06797812
H	1.87385893	1.94035950	-0.93635160
H	-0.16806306	2.60370622	2.38501389
H	-1.40297718	1.04227923	-1.21120976
H	-0.02039123	-3.39985982	2.80010414
H	-0.24281545	-3.95401563	1.10544470
H	-1.60740877	-3.19627868	1.98161886
H	-3.49843404	1.08195837	2.39225320
H	-2.51475208	2.53448689	2.02234737
H	-1.99914865	1.40242328	3.32029071

X-ray diffraction structures (ORTEP) of the reaction products 3a and 5b.



3a



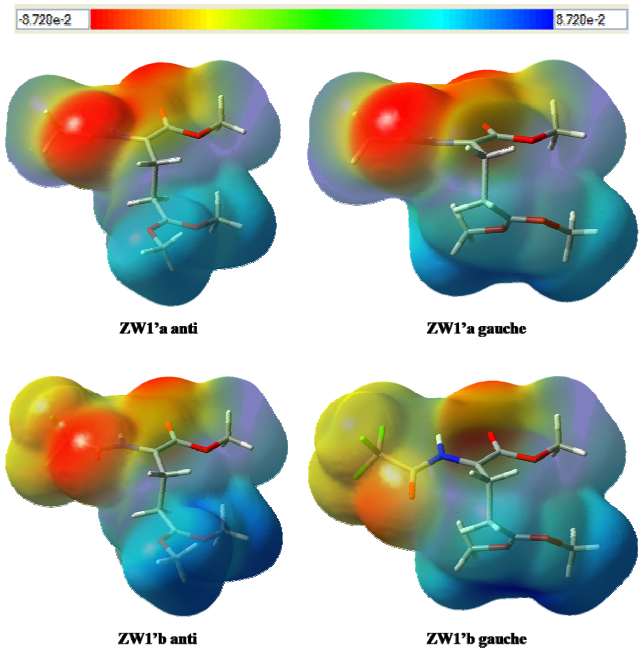
5b

50% probability chosen for the ellipsoids

Crystal data for compound **3a**: see reference "A. Avenoza, J. H. Busto, N. Canal and J. M. Peregrina, *Chem. Commun.*, 2003, 1376". CIF data for CCDC-204647 (**3a**) can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax: (+44)1223-336-033; or deposit@ccdc.cam.ac.uk).

Crystal data for compound **5b**: CIF data for CCDC-294888 (**5b**) can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax: (+44)1223-336-033; or deposit@ccdc.cam.ac.uk).

Electrostatic potential (ESP) surfaces of 1,4-zwitterionic intermediates



Electrostatic potential (ESP) surfaces of 1,4-zwitterionic intermediates calculated at the PCM/B3LYP/6-31+G(d) level. ESP are plotted on the Total Density Isosurface at a value of 0.0004 e·Bohr^{-3}, and the displayed ranges are given in Hartrees at the top of the figure.