Supporting information to

Origin of the Asymmetric Induction in the Metallosalen-catalysed Reactions of Aldehydes

*Wojciech Chaładaj and Janusz Jurczak**

1 Table of contents

2 Experimental part

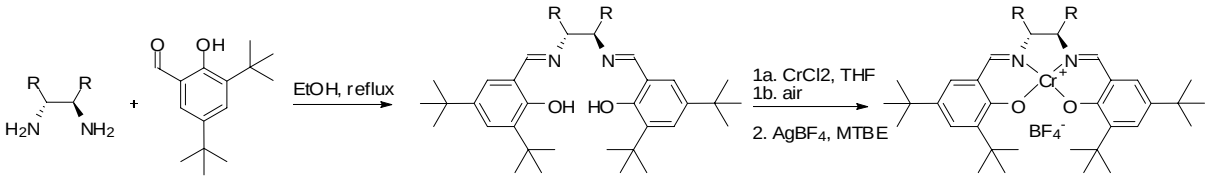
2.1 General

All reported NMR spectra were recorded in $CDCl_3$ using a Bruker spectrometer at 500 MHz (^{1}H NMR) and 125 MHz (^{13}C NMR). Chemical shifts of ^{1}H NMR and ^{13}C NMR are reported as δ values relative to TMS (δ=0.00) and $CDCl_3$ (δ=77.0), respectively. The following abbreviations were used to indicate the multiplicity: s, singlet; brs, broad singlet; d, doublet; m, multiplet; coupling constants are reported in Hz. High resolution mass spectra (HRMS) were performed on Mariner unit using the ESI technique. Optical rotations were measured employing a JASCO P-2000 polarimeter. Analytical TLC was carried out on commercial plates coated with 0.25 mm of Merck Kieselgel 60. Preparative flash silica chromatography was performed using Merck Kieselgel 60 (230-400 mesh). Enantiomeric excesses of the products were determined using Trace 2000 GC (Thermo Finnigan) apparatus equipped with a flame ionization detector (FID) and a capillary chiral β-dex 120 column (permethyl-β-cyclodextrin, 30 m x 0.25 mm I.D. Supelco, Bellefonte, USA) employing nitrogen as a carrier gas. Data were acquired under the following conditions: pressure of nitrogen- 100 kPa, injector temperature - 210°C, detector temperature - 250°C. Oven temperature varied according to cycloadducts (*vide infra*).

All commercially available chemicals were used as received unless otherwise noted.

2.2 Synthesis of catalysts 1a-1e

Catalyst **1a-1d** were synthesized in analogical way as classic Jacobsen complex **1a**:



2a R=-$(CH_2)_4$-
2b R= Ph
2c R= Me
2d R= *c*-C_6H_{11}
2e R= *t*-Bu

3a R=-$(CH_2)_4$-
3b R= Ph
3c R= Me
3d R= *c*-C_6H_{11}
3e R= *t*-Bu

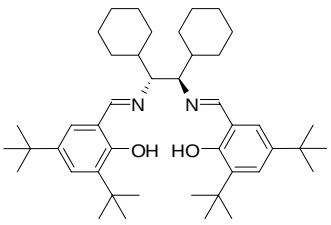
1a R=-$(CH_2)_4$-
1b R= Ph
1c R= Me
1d R= *c*-C_6H_{11}
1e R= *t*-Bu

Homochiral diamines **2a-e** were either commercially available (**2a** and **2b**) or synthesized according to literature procedures - **2c**,[1] **2d**,[2] **2e**.[3] Ligand **3a** is commercially available and was used as received. Ligand **3b** was synthesized according to known procedure.[4] Compounds **3c-3d** were synthesized by condensation of appropriate amine with 3,5-di-*tert*-butylsalicylaldehyde following the procedure for **3b**. Catalysts **1a-e** were obtained from salen ligands **3a-e** employing the Jacobsens procedure for **1a**.[5]

General procedure for synthesis of salen ligands 3c-3e. To the solution of diamine (1 mmol) in ethanol (5 ml) 3,5-di-*tert*-butylsalicylaldehyde (468mg, 2 mmol) was added at 60 ºC and the resulting mixture was heated in reflux for 3h. Afterwards water (1 ml) was added and the mixture was cooled to 4 ºC. Yellow crystals were filtered, dried under vacuum yielding desired product **3**.

(S,S)-N,N'-Bis(3,5-di-tert-butylsalicylidene)-butane-2,3-diamine (3c) yield: 92%, mp=148-149ºC; $[\alpha]^{rt}_D$= +208.5 (c=0.59, $CHCl_3$); ^{1}H NMR 1.26 (s, 18H), 1.37 (d, J=6.0, 6H), 1.42 (s, 18H), 3.43-3.51 (m, 2H), 7.02 (d, J=2.4, 2H), 7.32 (d, J=2.4, 2H), 8.32 (s, 2H), 13.66 (s, 2H); ^{13}C NMR 18.9, 29.4, 31.4, 34.1, 35.0, 69.4, 117.8, 126.0, 126.8, 136.5, 139.9, 158.1, 165.4; IR (KBr) ν; 2995, 2953, 2869, 1630, 1594; HRMS: $[M+Na]^+$ calcd for $C_{34}H_{52}N_2O_2Na$: 543.39210, found: 543.38969.

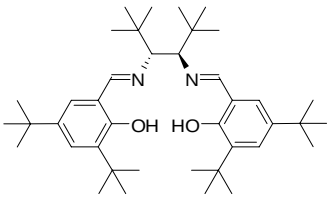
(R,R)-N,N'-Bis(3,5-di-tert-butylsalicylidene)-1,2-dicyclohexylethane-1,2-diamine (3d)



yield: 91%, mp= 147-150 ºC; $[\alpha]^{rt}_D$=-86.0 (c=0.56, $CHCl_3$); ^{1}H NMR 1.01-1.34 (m, 8H), 1.24 (s, 18H), 1.42 (s, 18H), 1.53-1.81 (m, 12H), 3.29-3.33 (m, 2H), 6.96 (d, J=2.4, 2H), 7.30 (d, J=2.4, 2H), 8.14 (s, 2H), 13.78 (s, 2H); ^{13}C NMR 26.3, 26.4, 26.4 27.9, 29.4, 31.2, 31.4, 34.0, 35.0, 38.3, 75.1, 117.7, 126.0, 126.6, 136.4, 139.5, 158.3, 166.2; IR (KBr) ν 2955, 2930, 2854, 1626, 1596; HRMS: $[M+H]^+$ calcd for $C_{44}H_{69}N_2O_2H$: 657.53536, found: 657.53681.

[1] S. Y. M. Chooi, P. LEung, S. Ng, G. H. Quek, K. Y. Sim, *Tetrahedron: Asymmetry* 1991, **2**, 981.
[2] S. E. Denmark, X. Su, Y. Nishigaichi, D. M. Coe, K.-T. Wong, S. B. D. Winter, J. Y. Choi, *J. Org. Chem.* 1999, **64**, 1958
[3] S. Roland, P. Mangeney, A. Alexakis, *Synthesis* 1999, 228.
[4] P. Pietikäinen, *Tetrahedron* 2000, **56**, 417.
[5] S. E. Schaus, J. Brånalt, E. N. Jacobsen, *J. Org. Chem.* 1998, **63**, 403.

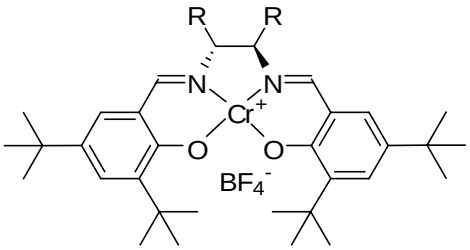
(R,R)-N,N'-Bis(3,5-di-tert-butylsalicylidene)-2,2,5,5-tetramethylhexane-3,4-diamine (3e)



yield: 87%; mp= 269-270 ºC; $[\alpha]^{rt}_D$=+125.2 (c= 0.52, $CHCl_3$); ^{1}H NMR 0.92 (s, 18H), 1.33 (s, 18H), 1.43 (s, 18H), 3.38 (s, 2H), 7.12 (d, J= 2.4, 2H), 7.40 (d, J= 2.4, 2H), 8.42 (s, 2H), 13.69 (s, 2H); ^{13}C NMR 27.9, 29.5, 31.6, 34.1, 35.1, 36.1, 77.8, 117.6, 125.8, 127.0, 137.0, 139.3, 158.8, 166.5; IR (KBr) ν 2963, 2908, 2871, 1628, 1596; HRMS: $[M+H]^+$ calcd for $C_{40}H_{65}N_2O_2H$: 605.50406, found: 605.50274.

Catalysts 1a-e

Chromium(II) chloride (123 mg, 1mmol) and salen ligand **3** (0.8 mmol) in dry degassed THF (10 ml) was stirred for 3h under argon and further 3h under air atmosphere. After that time the mixture was diluted with MTBE (40 ml) and washed with saturated NH_4Cl solution (5x30ml), brine (3x 30ml), dried with $MgSO_4$ and concentrated. The resulting brown solid was dissolved in MTBE/CH_2Cl_2 (20/10 ml), $AgBF_4$ (0.8 mmol) was added and the reaction flask was wrapped with aluminum foil. The mixture was stirred overnight, filtered through the pad of cellite and concentrated. The brown solid was dried at 80 ºC under high vacuum for 1h yielding complexes **1** in quantitative (or nearly quantitative) yield. Complexes were used without purification.



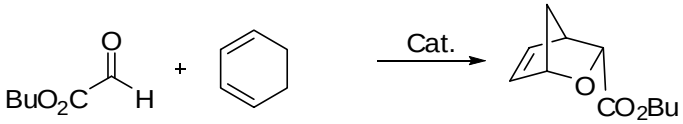
HRMS: $[M - BF_4]^+$

Cat.	$[M - BF_4]^+$	calcd.	found
1b	$C_{44}H_{54}N_2O_2Cr$	694.35849	694.35714
1c	$C_{34}H_{50}N_2O_2Cr$	570.32719	570.32471
1d	$C_{44}H_{66}N_2O_2Cr$	706.45558	706.45342
1e	$C_{40}H_{62}N_2O_2Cr$	654.42109	654.4243

2.3 Model Reactions

n-Butyl glyoxylate was prepared by oxidative cleavage of appropriate tartrate ester using $NaIO_4$ in water[6] and distilled under reduced pressure (ca. 20 mm Hg) in the presence of P_2O_5 prior to use.

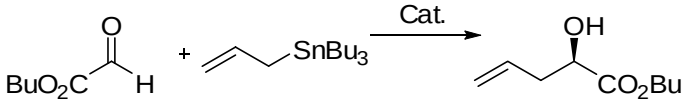
Reaction 1. Cycloaddition of cycloxexa-1,3-diene to n-butyl glyoxylate.[7]



To a solution of catalyst (0.01 mmol) and n-butyl glyoxylate (130 mg, 1 mmol, freshly distilled from P_2O_5) in toluene (1 ml) cycloxexa-1,3-diene (75 μl, 62 mg, 1.5 mmol) was added, and the solution was stirred for 24 hour at rt. The reaction mixture was directly subjected to column chromatography (hexane:AcOEt 8:2) yielding desired product. Afterwards the enantiomeric excess of product was determined by GC analysis of the reaction mixture: temp= 160ºC, $t_{r(S)}$= 33.1, $t_{r(R)}$=34.1

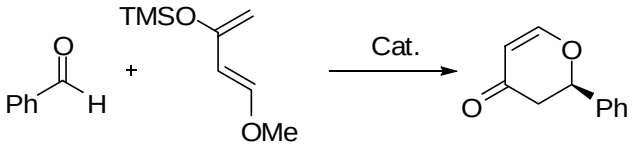
[6] M. A. Brimble, M. K. Edmonds, *Synth. Commun*. 1996, **26**, 243.
[7] P. Kwiatkowski, M. Asztemborska, J.-C. Caille, J. Jurczak, *Adv. Synth. Catal.* 2003, **345**, 506.

Reaction 2. Addition of allyltributylstannane to n-butyl glyoxylate. [8]



To a solution of catalyst (0.02 mmol) and n-butyl glyoxylate (130 mg, 1 mmol, freshly distilled from P_2O_5) in dichloromethane (1 ml) allyltributylstannane (365 mg, 1.1 mmol) was added dropwise, and the solution was stirred for 3 hours at rt. Afterwards the reaction mixture was diluted with wet Et2O, dried with $MgSO_4$ and subjected to column chromatography (hexane:AcOEt 9:1) yielding desired product. The enantiomeric excess of product was determined by GC analysis of the reaction mixture: temp.=130ºC, $t_{r(R)}$= 13.6, $t_{r(S)}$=14.1.

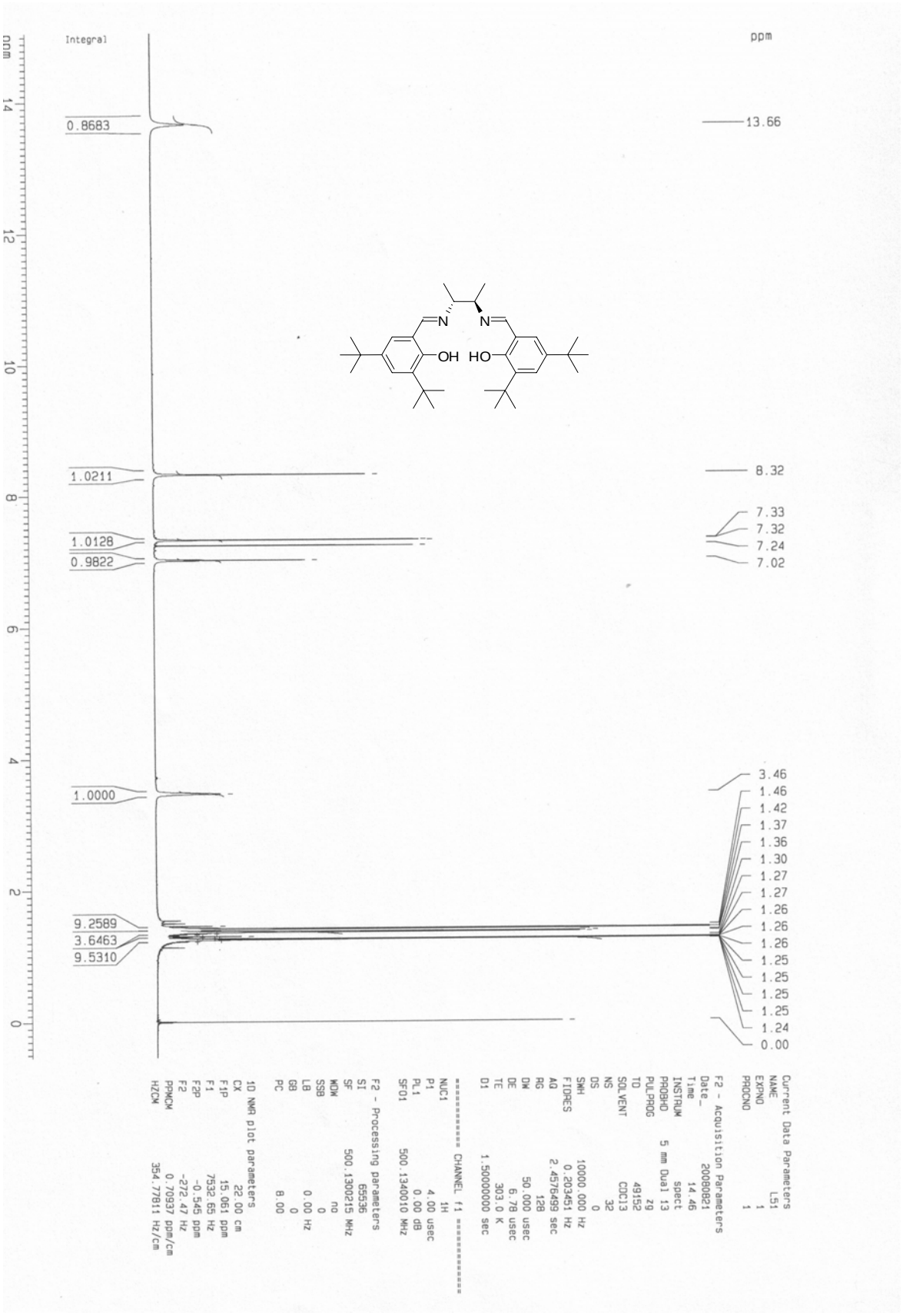
Reaction 3. Reaction of Danishefsky's diene with benzaldehyde. [5]

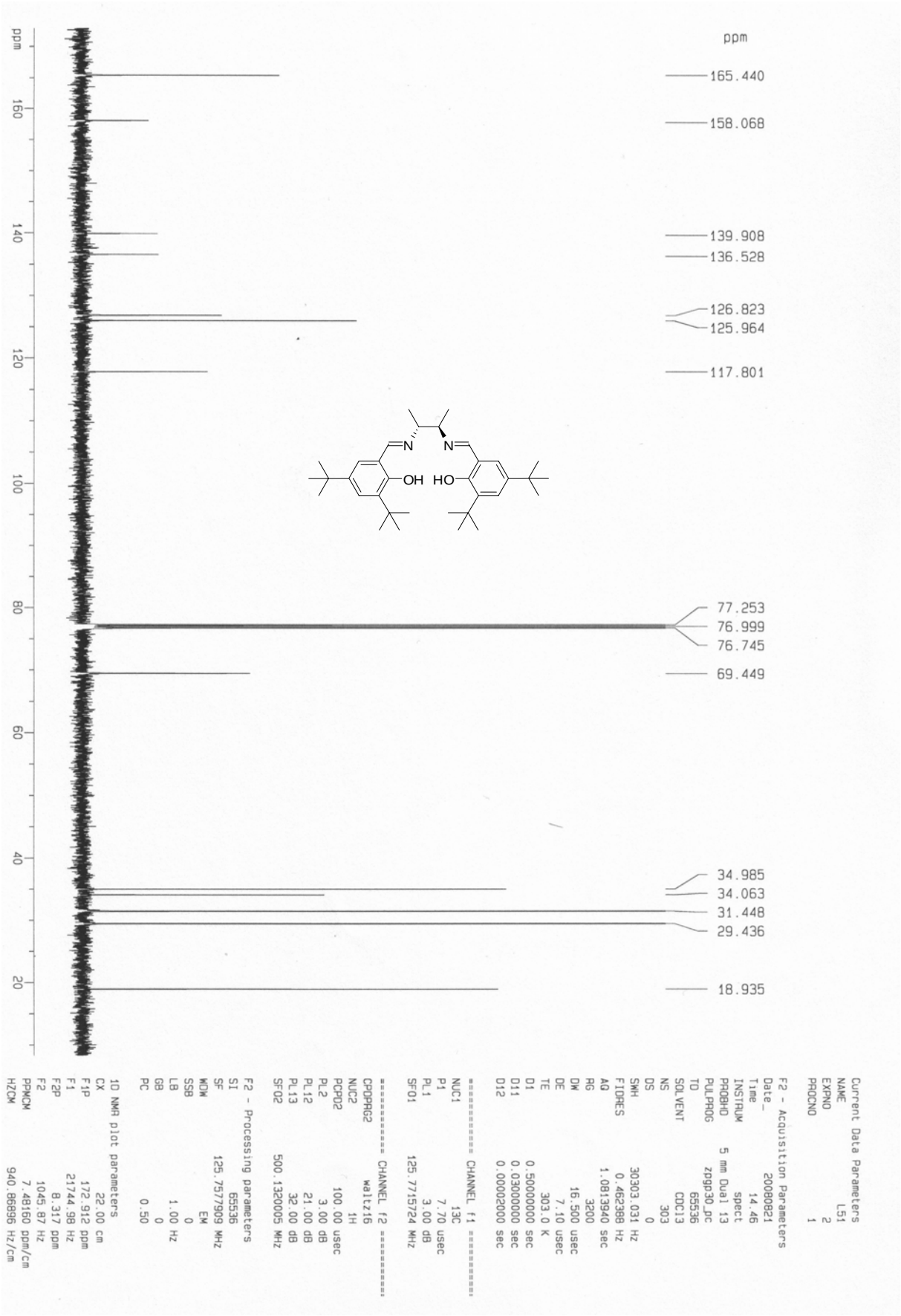


To a mixture of catalyst (0.02 mmol), benzaldehyde (106 mg, 1 mmol) and molecular sieves 4A (300mg) in MTBE (200µl) at -30 ºC Danishefsky's diene (195 µl, 172 mg, 1 mmol) was added dropwise, and the reaction mixture was stirred for 24 hour at -30 ºC. Afterwards the reaction mixture was diluted with dichloromethane (ca. 3ml), trifluoroacetic acid was added (two drops) and after stirring for 10 minutes it was filtered through the pad of Celite, washed with $NaHCO_3$, dried with $MgSO_4$ and subjected to column chromatography (hexane:AcOEt 8:2) yielding desired product. The enantiomeric excess of product was determined by GC analysis of the reaction mixture: temp= 160ºC, $t_{r(S)}$= 32.2, $t_{r(R)}$=33.2.

[8] P. Kwiatkowski, W. Chaładaj, J. Jurczak, *Tetrahedron* 2006, **62**, 5116.

NMR spectra of ligands 3c-3e

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31.448
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HO
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D11 0.03000000 sec
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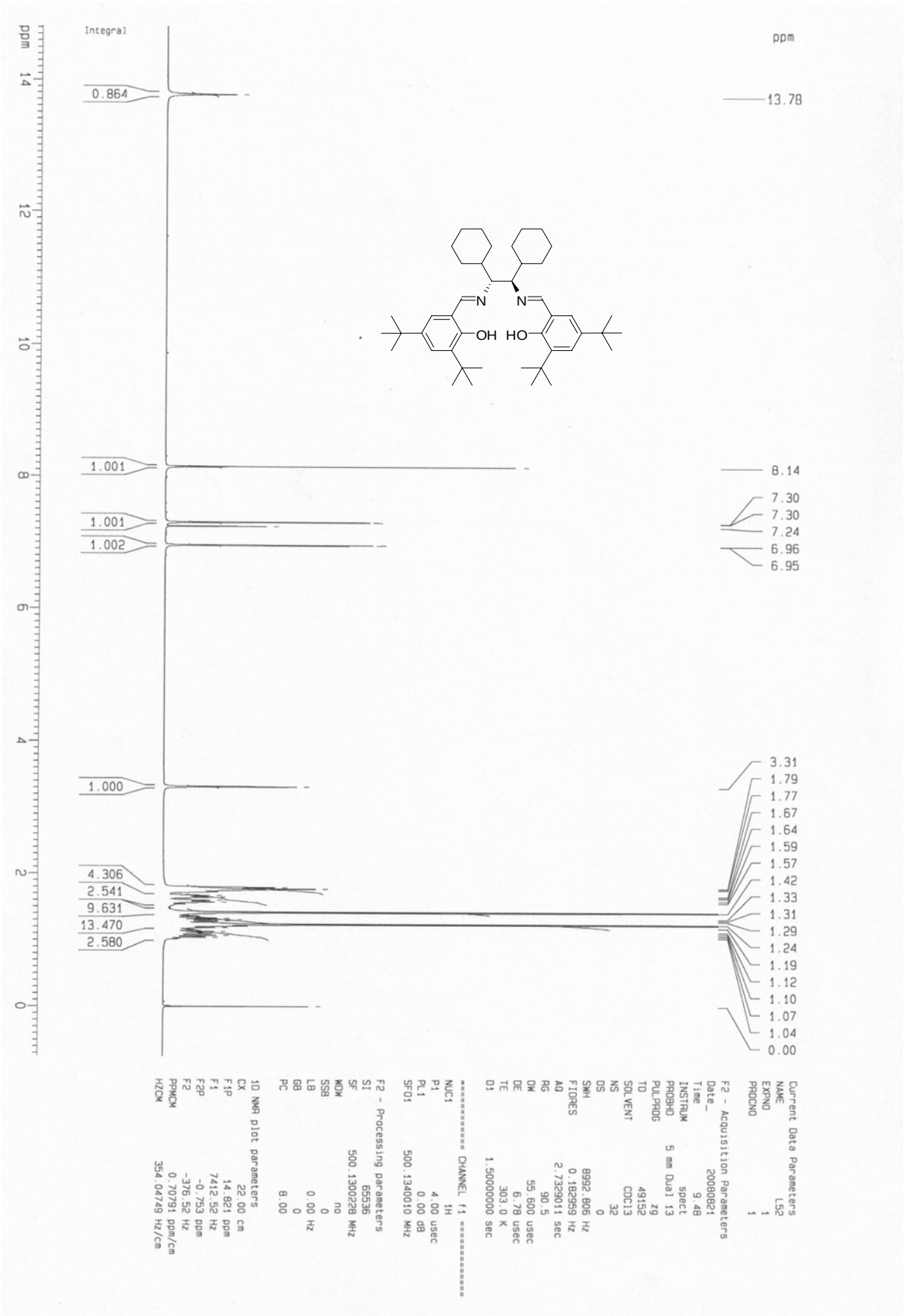
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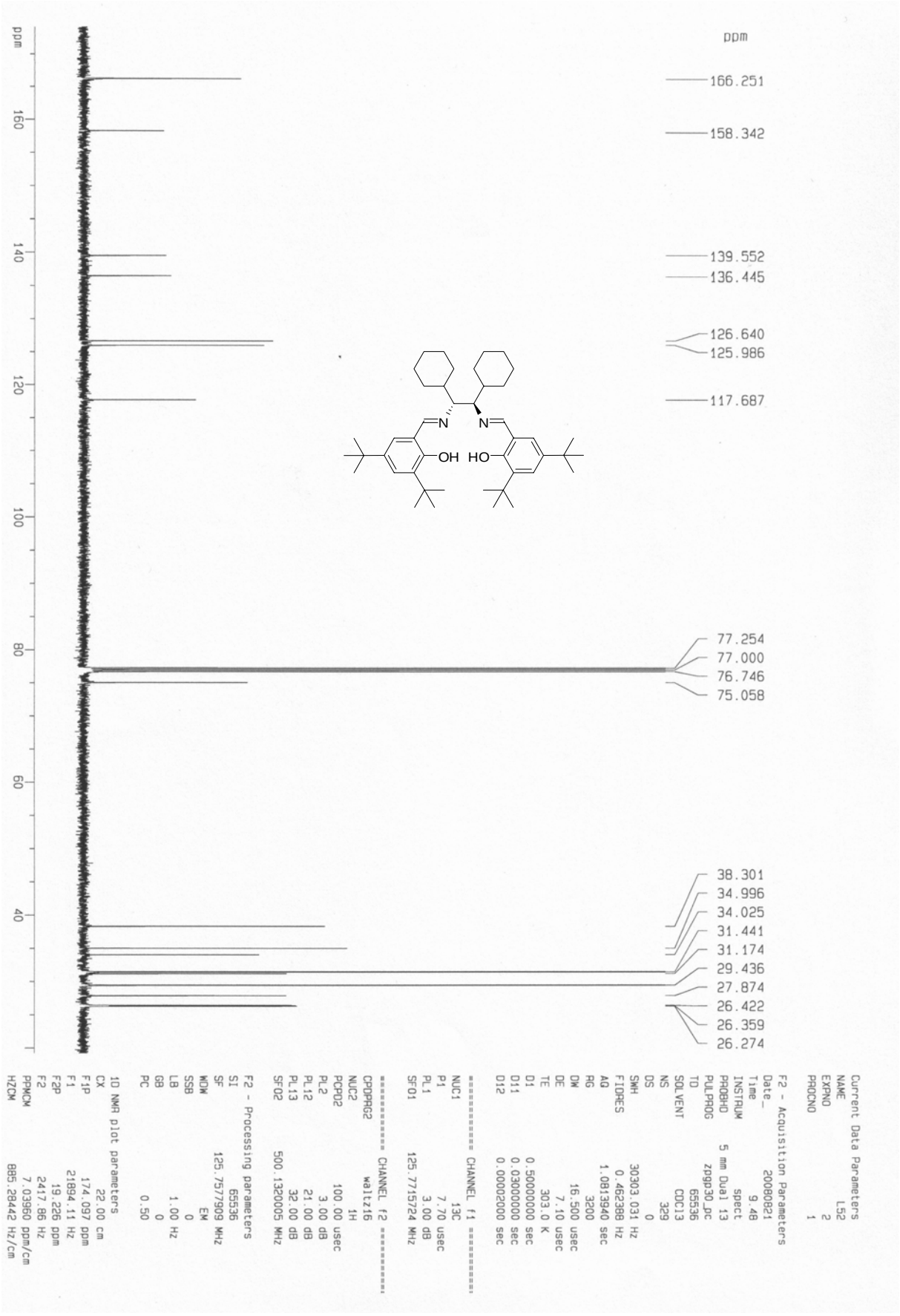
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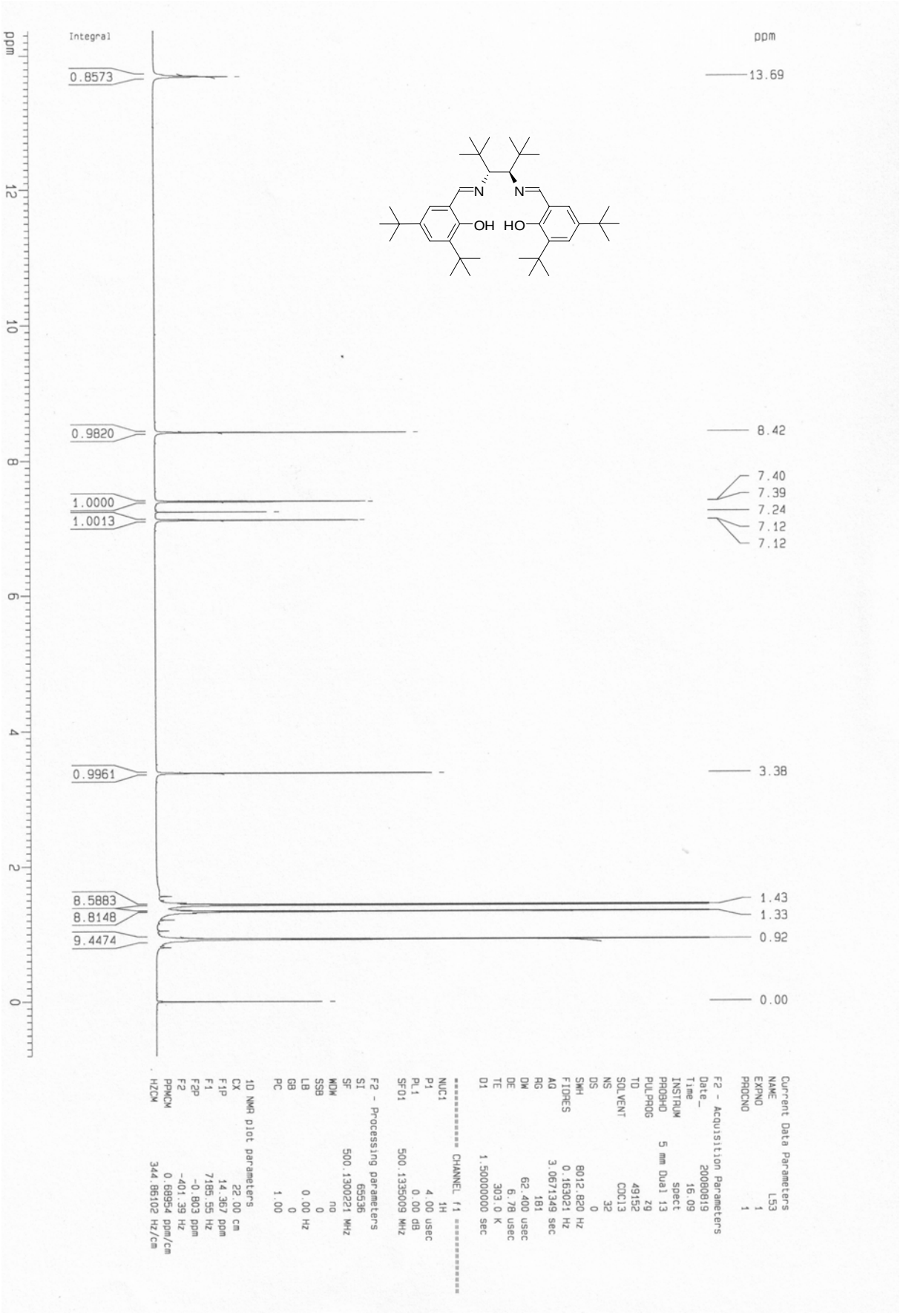
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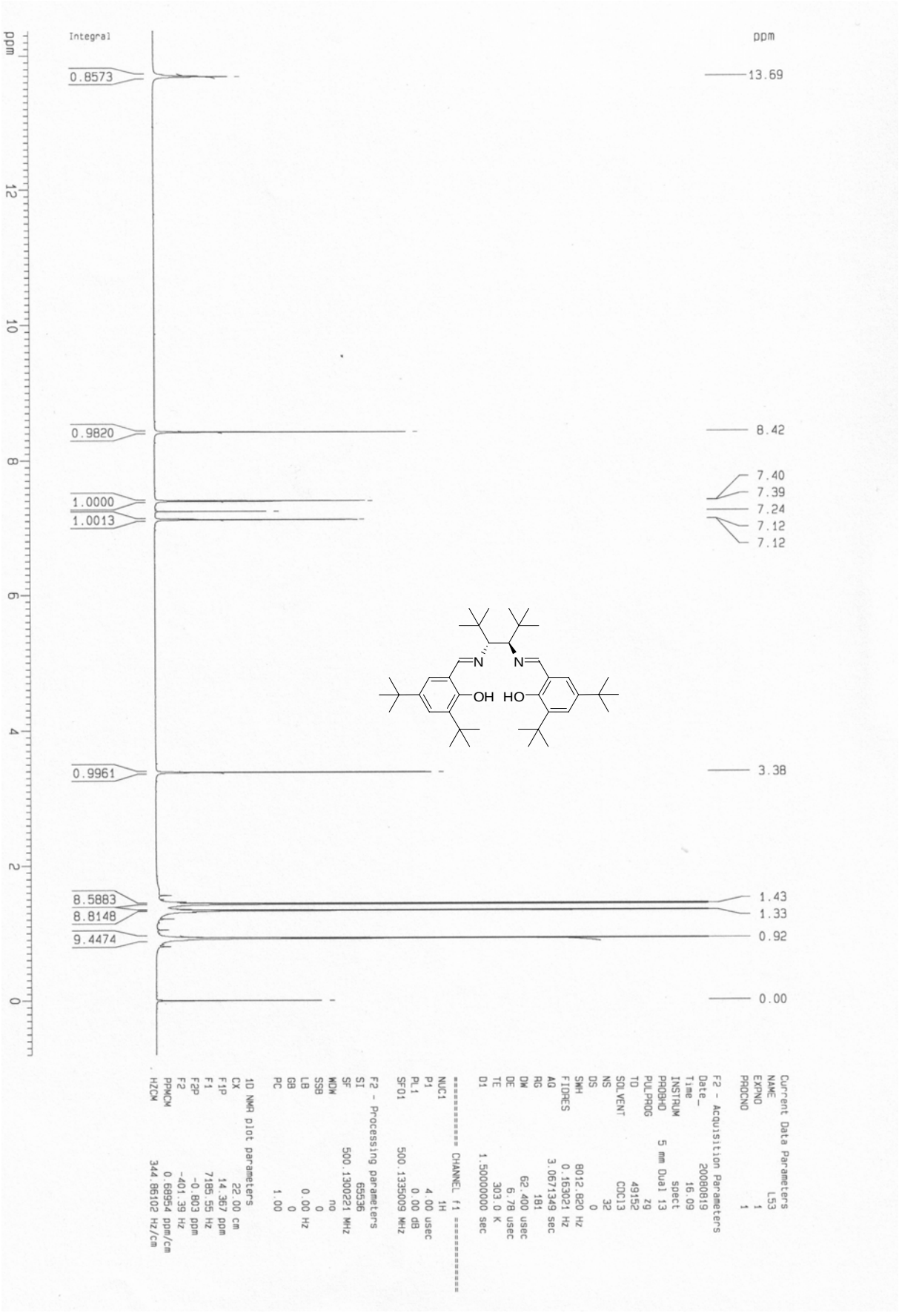
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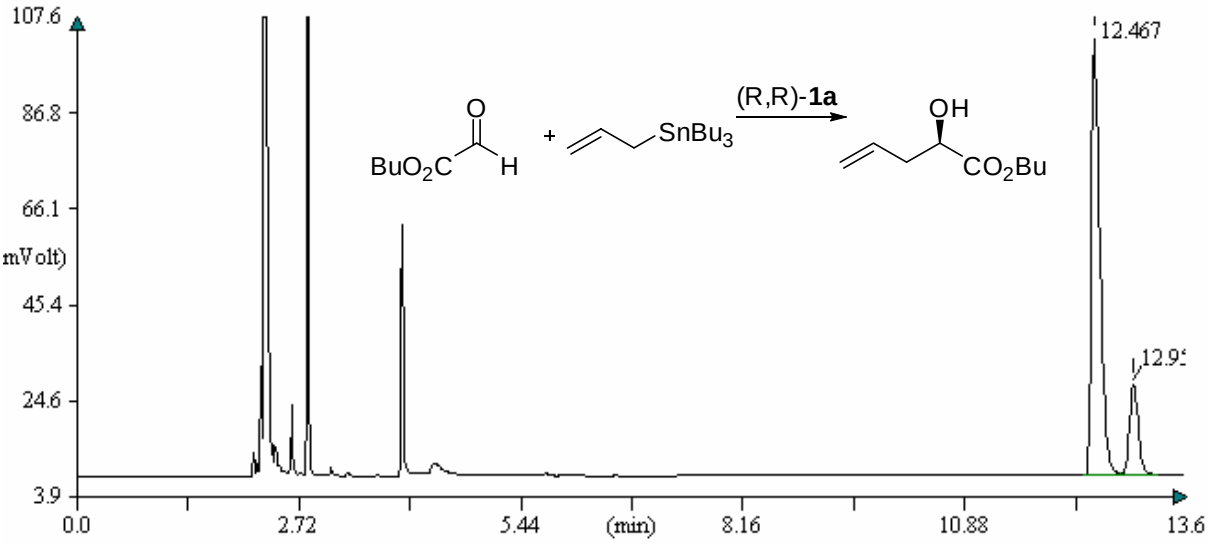
CX 22.00 cm
F1P 14.367 ppm
F1 7185.55 Hz
F2P -0.803 ppm
F2 -401.39 Hz
PPMCM 0.68954 ppm/cm
HZCM 344.86102 Hz/cm

2.4 GC chromatograms of model reactions



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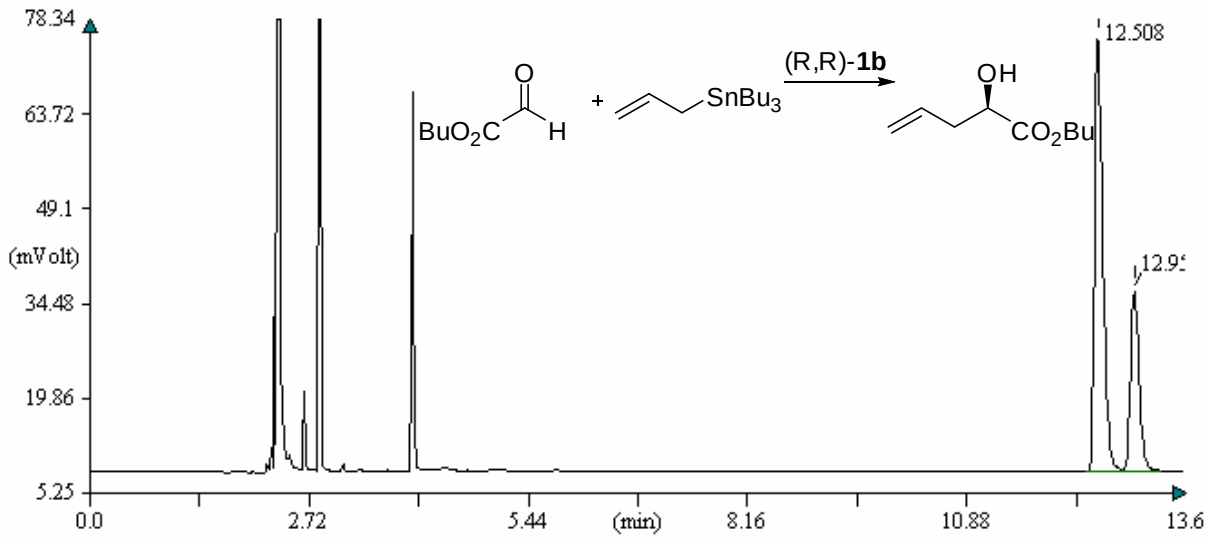

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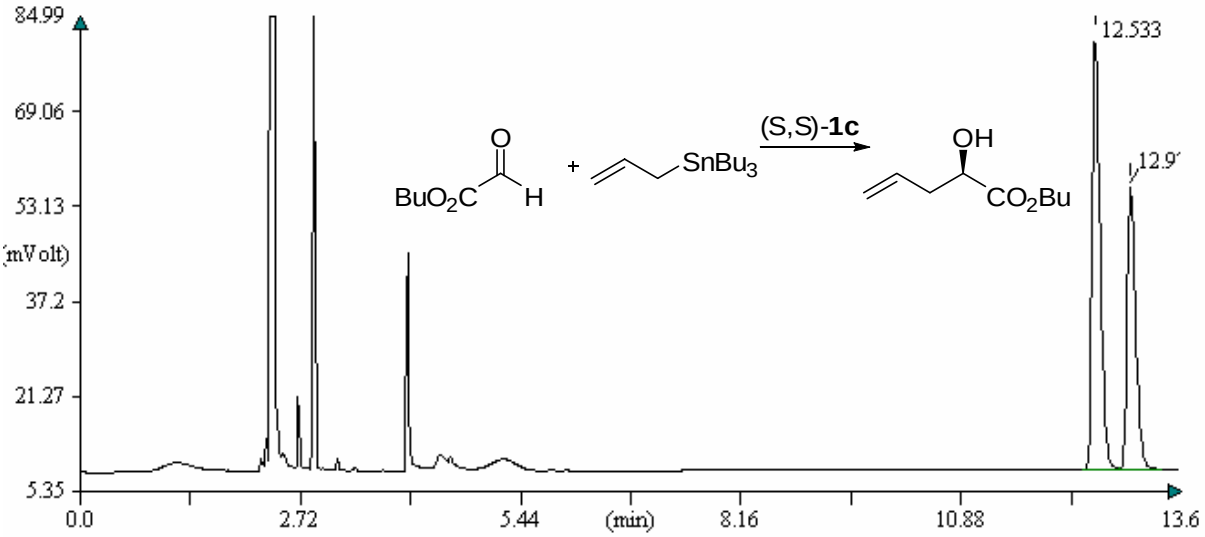

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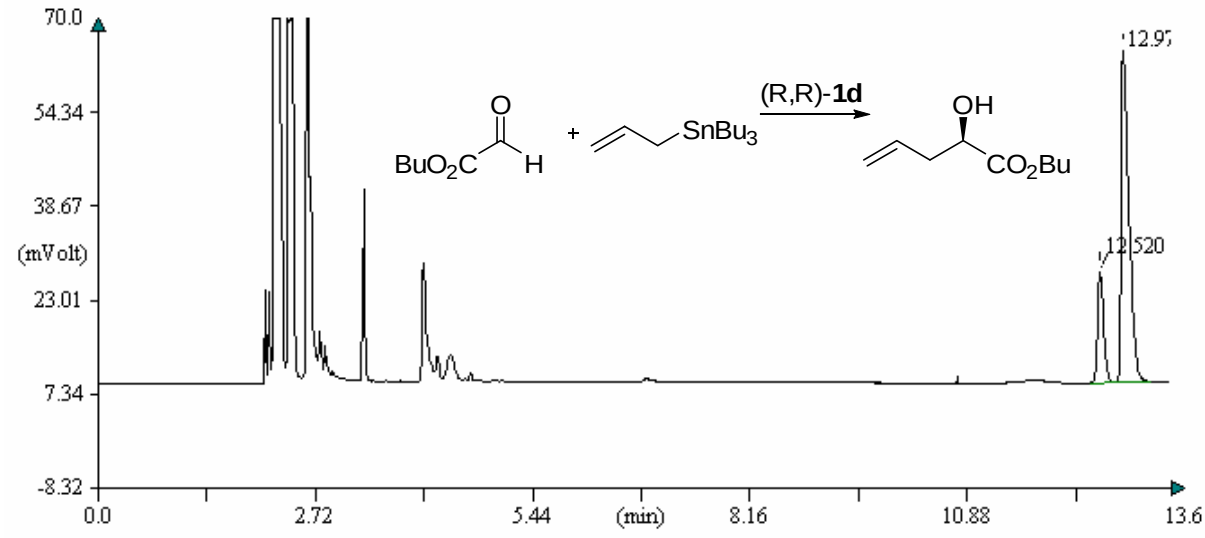
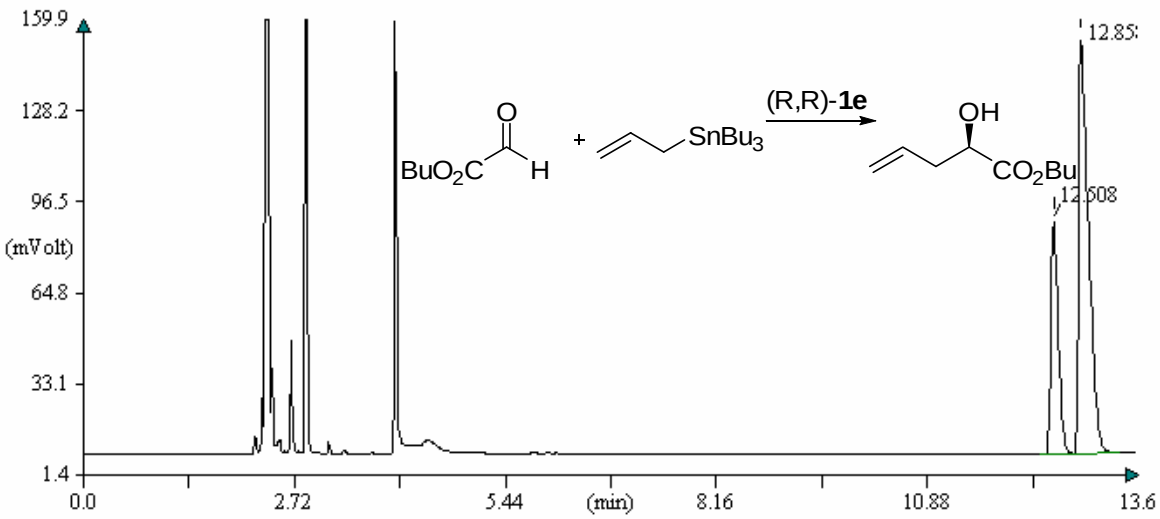
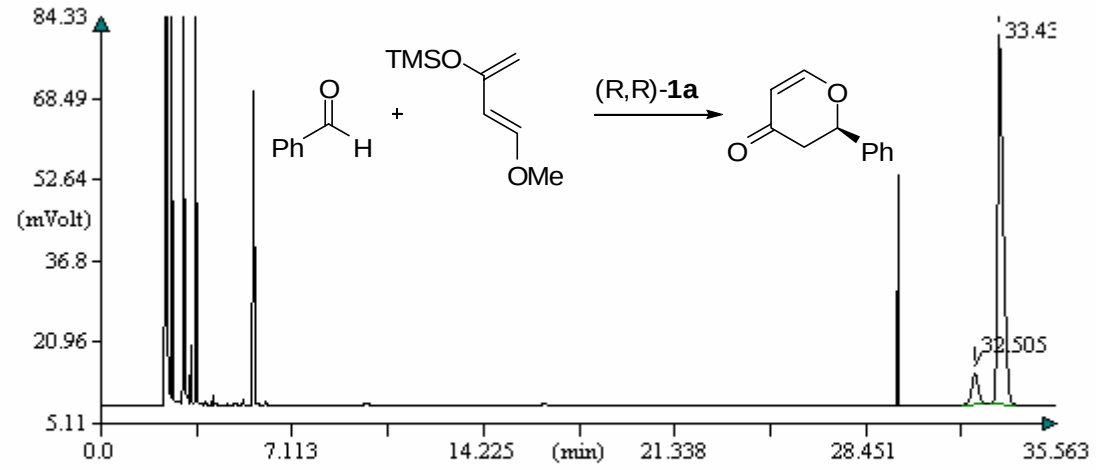


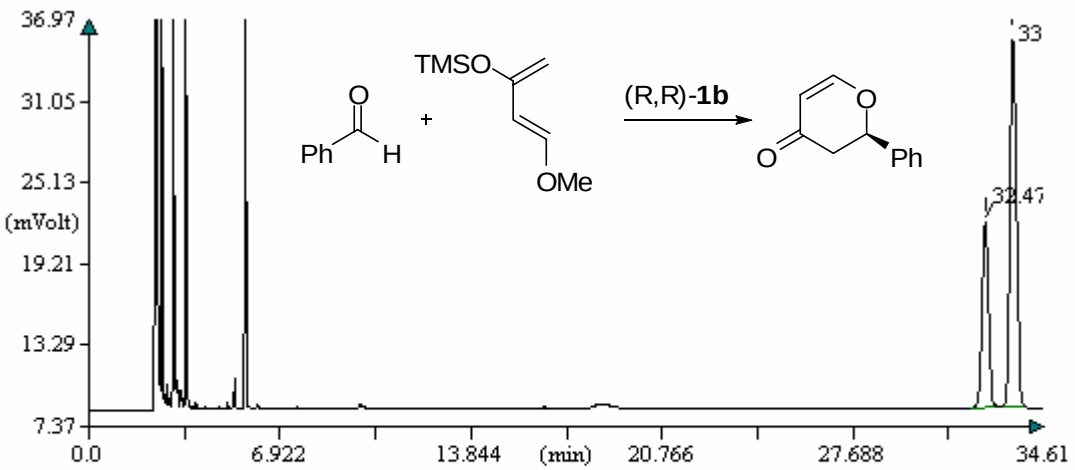
Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	12.520		20.578
2	12.970		79.422



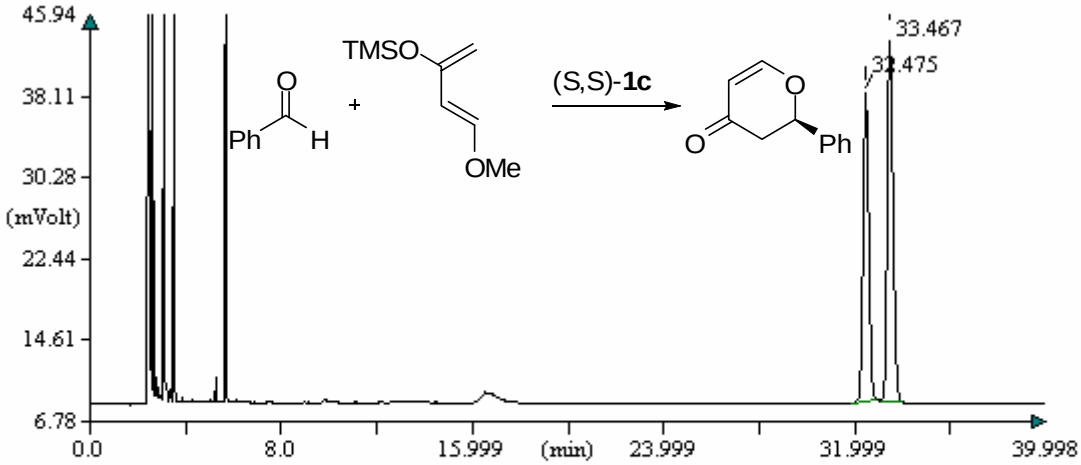
Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	12.508		29.305
2	12.858		70.695



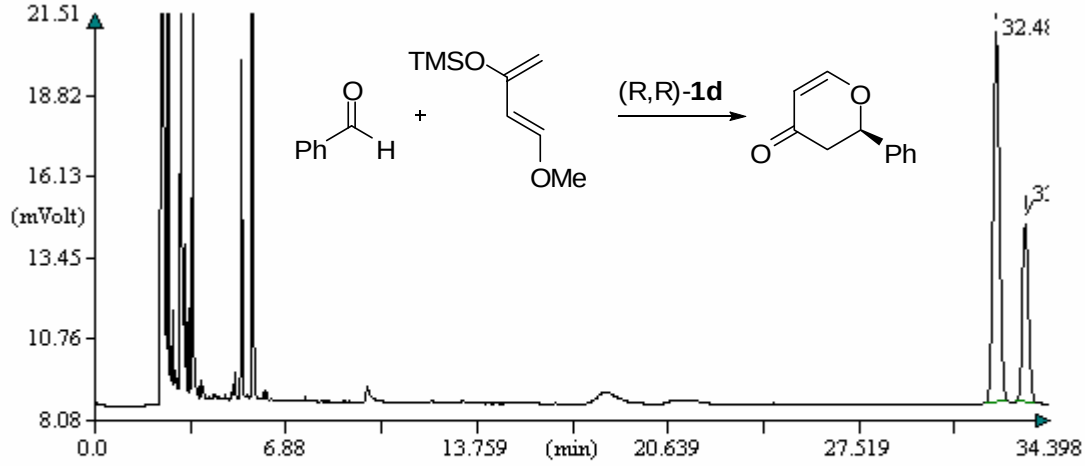
Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	32.505		7.329
2	33.435		92.671



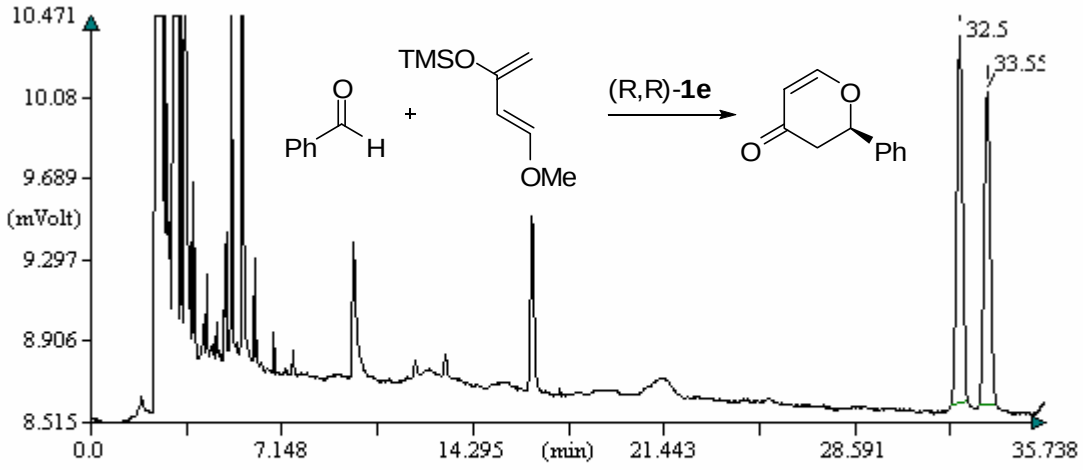
Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	32.475		32.878
2	33.475		67.122



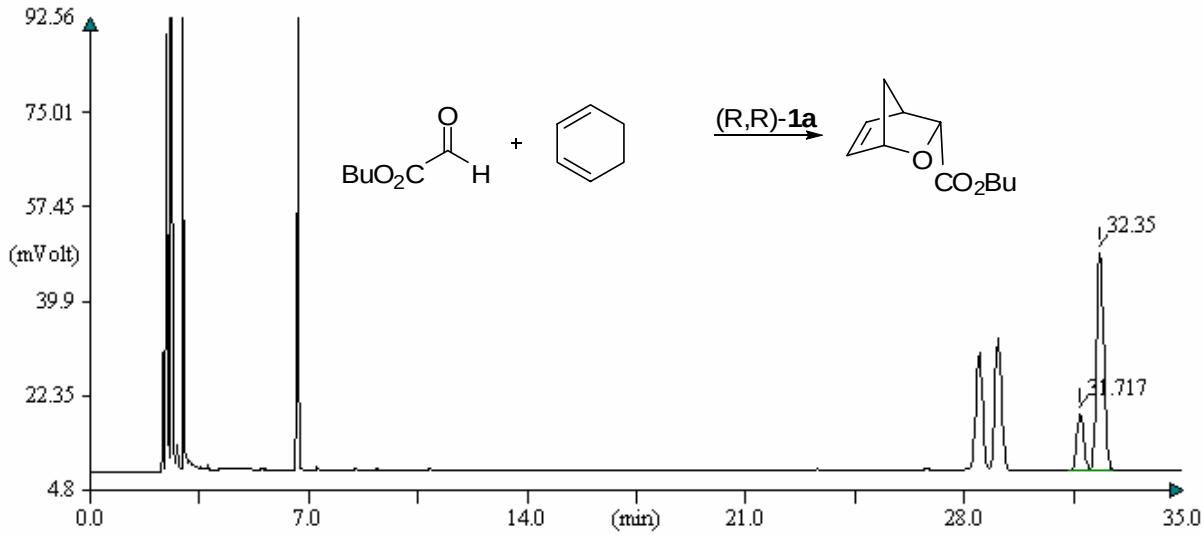
Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	32.475		45.608
2	33.467		54.392



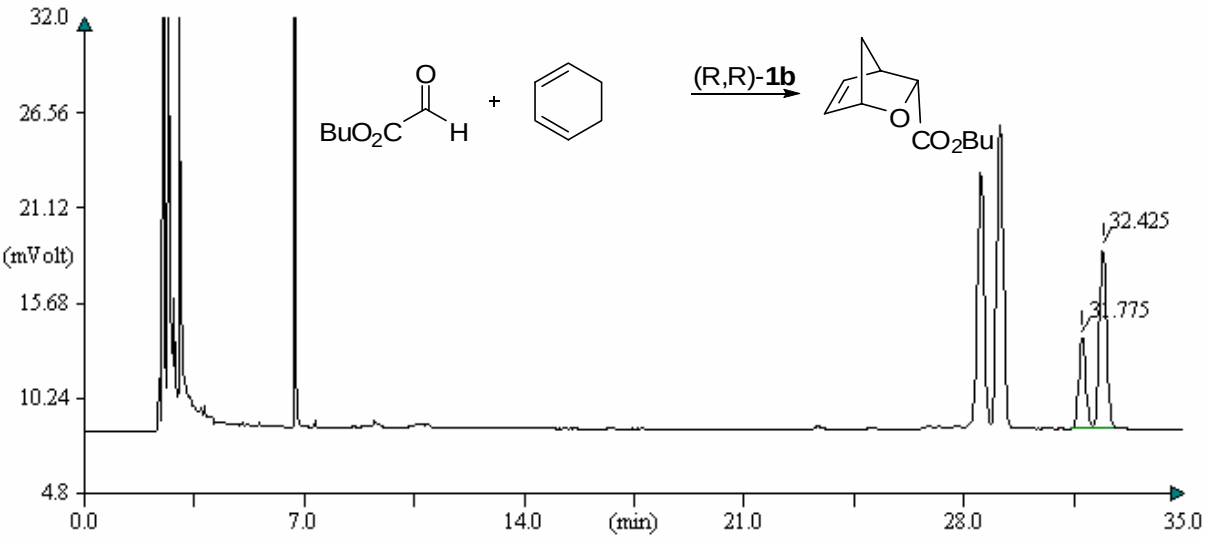
Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	32.480		66.913
2	33.520		33.087



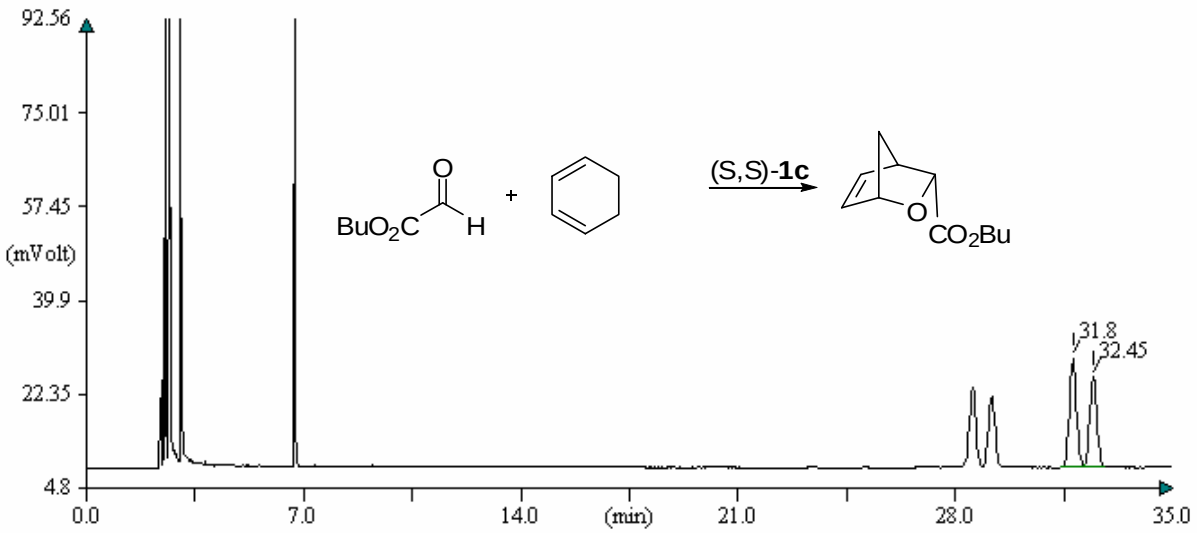
Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	32.500		53.226
2	33.550		46.774



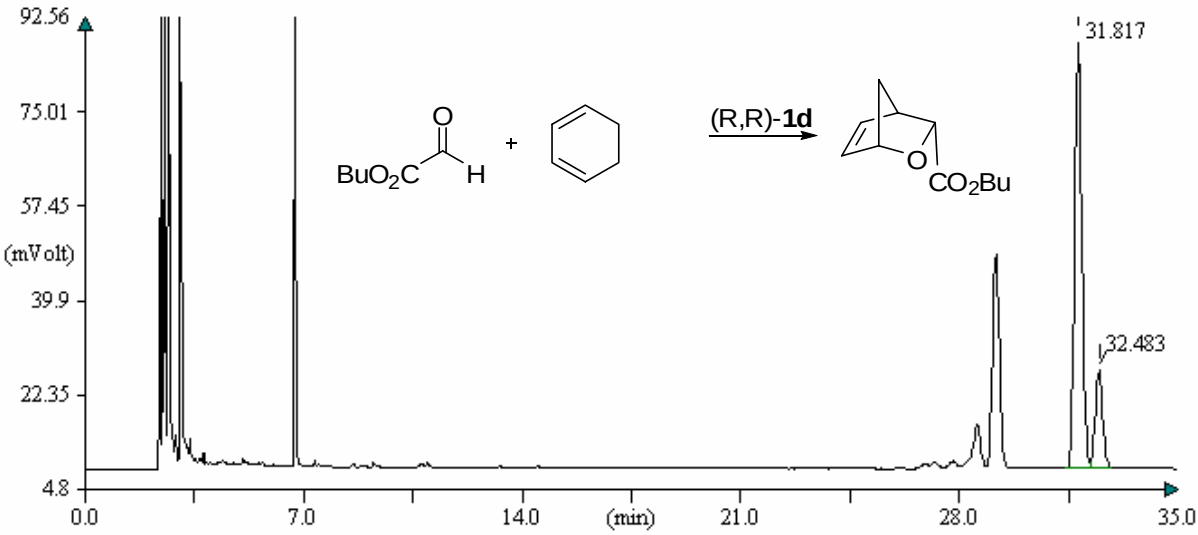
Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	31.717		20.125
2	32.350		79.875



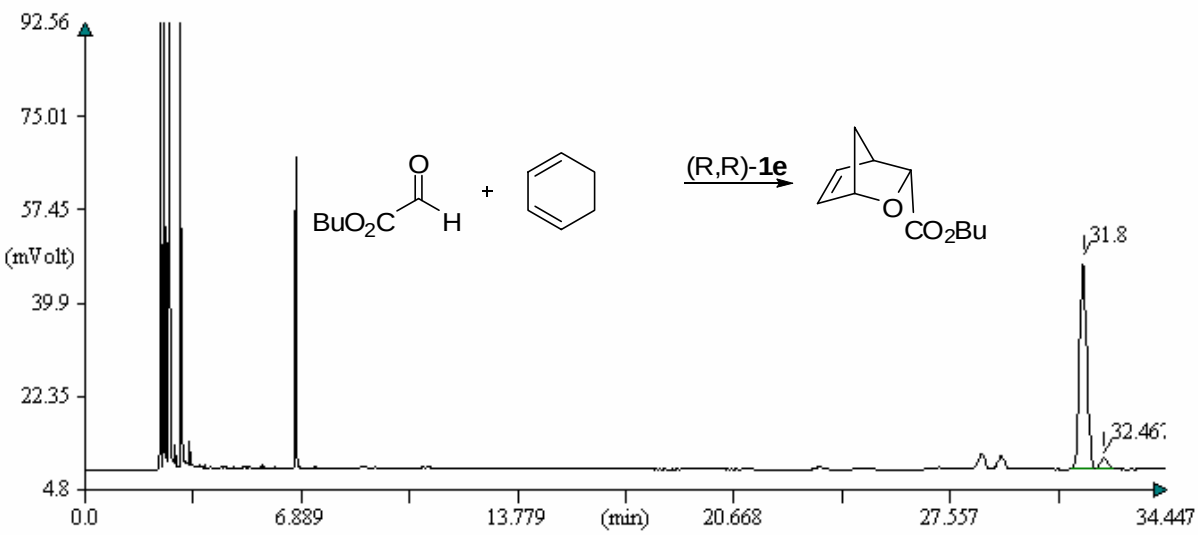
Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	31.775		32.880
2	32.425		67.120



Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	31.800		54.451
2	32.450		45.549



Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	31.817		81.212
2	32.483		18.788



Peak Number (#)	Retention Time (min)	Component Name	Area % (%)
1	31.800		95.438
2	32.467		4.562

3 Computational part

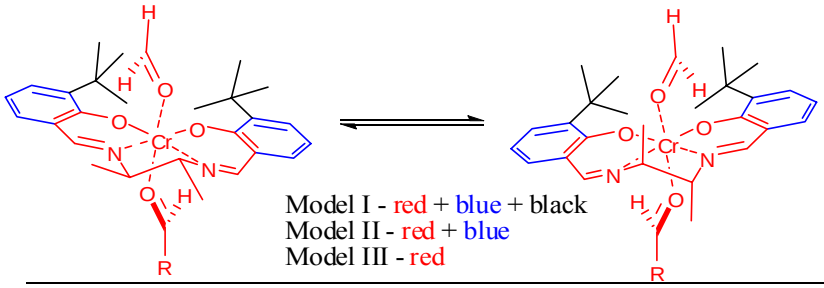
3.1 General

All calculations were performed with Gaussian 03 revision B.05 or E.01.[9] Geometries were optimized at given level of theory (usually B3LYP/6-31G(d)) and the nature of the stationary points was confirmed frequencies by frequency calculations - 0 or 1 imaginary frequencies for ground and transition states, respectively. Corrections to thermodynamic functions were calculated for standard conditions (298.15K, 1.0 atm.) and were not scaled. Chromium complexes were calculated as quartets. Doublet and sextet spin states of investigated chromium complexes were higher in energy by more than 100 kJ/mol. Energies are reported in atomic units.

3.2 Conformation of aldehyde-1c complex. Complexity of model and level of theory investigation

Influence of the model complexity.

Energies, ZPE correction and thermal corrections to thermodynamic functions calculated at B3LYP/6-31G(d).

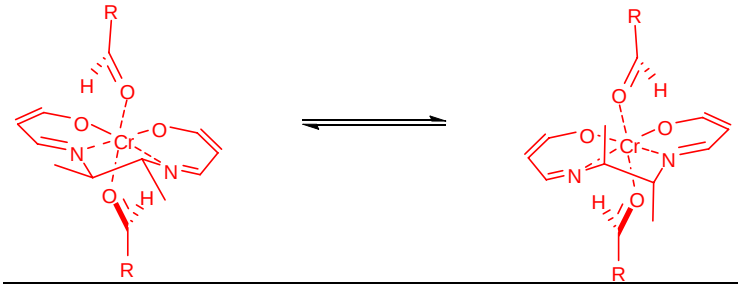


Level of Theory	Conformer	E	ZPE cor.	cor. to E	cor. to H	cor. to G
Model I	axial	-2544.61684317	0.615917	0.653413	0.654357	0.548327
Model I	equatorial	-2544.61362294	0.616190	0.653684	0.654628	0.547939
Model II	axial	-2230.11708214	0.389584	0.416052	0.416996	0.333380
Model II	equatorial	-2230.11368583	0.389750	0.416263	0.417207	0.332738
Model III	axial	-1922.81236216	0.295815	0.317088	0.318033	0.246398
Model III	equatorial	-1922.80905486	0.295885	0.317274	0.318218	0.245203

[9] M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004

Influence of the structure of aldehyde.

Energies, ZPE correction and thermal corrections to thermodynamic functions calculated at B3LYP/6-31G(d).



R in aldehyde	Conformer	E	ZPE cor.	cor. to E	cor. to H	cor. to G
Me	axial	-2001.48568818	0.351863	0.376370	0.377314	0.297271
Me	equatorial	-2001.48237279	0.352064	0.376587	0.377532	0.296719
Ph	axial	-2384.98419734	0.460347	0.490251	0.491195	0.396616
Ph	equatorial	-2384.98069301	0.460381	0.490383	0.491327	0.395081
t-Bu	axial	-2237.37663113	0.522585	0.554990	0.555934	0.457817
t-Bu	equatorial	-2237.37344320	0.522744	0.555201	0.556145	0.456672

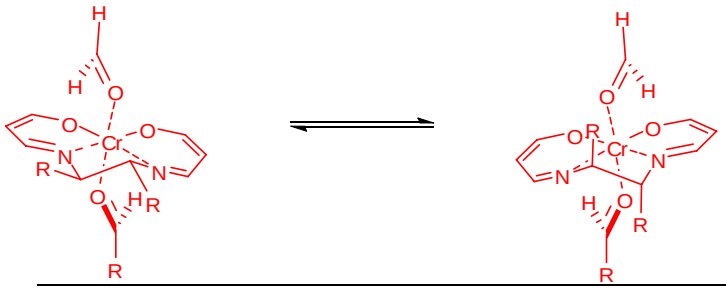
Influence of the functional used.

Energies, ZPE correction and thermal corrections to thermodynamic functions calculated at given level of theory for aldehyde-**1c** complex (Model III).

Level of Theory	Conformer	E	ZPE cor.	cor. to E	cor. to H	cor. to G
B3LYP/6-31G(d)	axial	-1922.81236216	0.295815	0.317088	0.318033	0.246398
B3LYP/6-31G(d)	equatorial	-1922.80905486	0.295885	0.317274	0.318218	0.245203
BLYP/6-31G(d)	axial	-1922.53773586	0.285867	0.307691	0.308635	0.236006
BLYP/6-31G(d)	equatorial	-1922.53448450	0.285901	0.307799	0.308743	0.235126
B3PW91/6-31G(d)	axial	-1922.41486771	0.296542	0.317828	0.318772	0.246933
B3PW91/6-31G(d)	equatorial	-1922.41231536	0.296768	0.318026	0.318970	0.246754
MPW1K/6-31G(d)	axial	-1922.54415332	0.305796	0.326542	0.327486	0.256857
MPW1K/6-31G(d)	equatorial	-1922.54134902	0.306075	0.326795	0.327739	0.256730
M05/6-31G(d)	axial	-1922.25508816	0.298296	0.319308	0.320252	0.249798
M05/6-31G(d)	equatorial	-1922.25140094	0.298914	0.319845	0.320790	0.249983

3.3 Conformation of aldehyde-catalyst complex

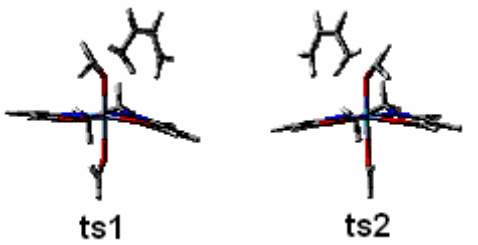
Energies, ZPE correction and thermal corrections to thermodynamic functions calculated at B3LYP/6-31G(d) level of theory for aldehyde-catalyst complex (Model III).



Cat.	R	Conformer	E	ZPE cor.	cor. to E	cor. to H	cor. to G
1b	Ph	axial	-2306.27321035	0.401432	0.429116	0.430060	0.341754
1b	Ph	equatorial	-2306.28395845	0.401223	0.429166	0.430111	0.340394
1c	Me	axial	-1922.81236216	0.295815	0.317088	0.318033	0.246398
1c	Me	equatorial	-1922.80905486	0.295885	0.317274	0.318218	0.245203
1d	*c*-C_6H_{11}	axial	-2313.53659159	0.542493	0.572702	0.573646	0.481173
1d	*c*-C_6H_{11}	equatorial	-2313.51847496	0.542983	0.573291	0.574235	0.480536
1e	*t*-Bu	axial	-2158.67252439	0.466334	0.495251	0.496195	0.409339
1e	*t*-Bu	equatorial	-2158.63441126	0.466557	0.495718	0.496662	0.409878

3.4 Transition states of (salen)Cr(III)-catalyzed HDA reaction

Energies, ZPE correction and thermal corrections to thermodynamic functions calculated at given level of theory for Model III transition states corresponding to approach of diene from *si* and *re* faces of aldehyde (ts1 and ts2, respectively)



Ts	Level of theory	E	ZPE cor.	cor. to E	cor. to H	cor. to G
ts1	B3LYP/6-31G(d)	-2000.16570160	0.329671	0.351872	0.352816	0.277633
ts2	B3LYP/6-31G(d)	-2000.16459520	0.329035	0.351584	0.352529	0.275888
ts1	MPW1K/6-31G(d)	-1999.86473611	0.339868	0.361981	0.362925	0.287685
ts2	MP1W1K/6-31G(d)	-1999.86313081	0.339566	0.360954	0.361898	0.288685
ts1	M05/6-31G(d)	-1999.54072778	0.329712	0.352867	0.353811	0.275851
ts2	M05/6-31G(d)	-1999.53935292	0.329408	0.351808	0.352752	0.277039

3.5 Coordinates of aldehyde-catalyst complexes optimized at B3LYP/6-31G(d)

Axial conformation of **1b**x2HCHO:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.246361	0.744091	-1.332418
2	6	0	0.246361	-0.744091	-1.332418
3	6	0	-0.266265	-2.581864	0.138428
4	6	0	0.266265	2.581864	0.138428
5	1	0	-0.352584	-3.174556	-0.776021
6	1	0	0.352584	3.174556	-0.776021
7	7	0	0.000000	1.303617	0.010624
8	7	0	0.000000	-1.303617	0.010624
9	24	0	0.000000	0.000000	1.530448
10	8	0	0.030671	-1.437213	2.849217
11	8	0	-0.030671	1.437213	2.849217
12	6	0	-0.419990	-3.267918	1.368579
13	1	0	-0.644137	-4.327328	1.332495
14	6	0	0.419990	3.267918	1.368579
15	1	0	0.644137	4.327328	1.332495
16	6	0	0.233460	2.684590	2.606650
17	1	0	0.299760	3.317718	3.496537
18	6	0	-0.233460	-2.684590	2.606650
19	1	0	-0.299760	-3.317718	3.496537
20	8	0	-2.055724	-0.096988	1.639725
21	8	0	2.055724	0.096988	1.639725
22	6	0	2.718761	-0.157530	2.638422
23	6	0	-2.718761	0.157530	2.638422
24	1	0	-2.248171	0.531346	3.556605
25	1	0	-3.806157	0.014658	2.607222
26	1	0	3.806157	-0.014658	2.607222
27	1	0	2.248171	-0.531346	3.556605
28	1	0	0.379054	1.298461	-2.041298
29	1	0	-0.379054	-1.298461	-2.041298
30	6	0	1.703401	-0.896711	-1.793514
31	6	0	2.077603	-0.359913	-3.035826
32	6	0	2.657088	-1.619633	-1.069436
33	6	0	3.371582	-0.520845	-3.527344
34	1	0	1.350969	0.176974	-3.641613
35	6	0	3.956017	-1.781012	-1.560192
36	1	0	2.391356	-2.073733	-0.121539
37	6	0	4.320039	-1.229459	-2.786705
38	1	0	3.635776	-0.099108	-4.492798
39	1	0	4.680620	-2.347902	-0.981984
40	1	0	5.328425	-1.357786	-3.168740
41	6	0	-1.703401	0.896711	-1.793514
42	6	0	-2.077603	0.359913	-3.035826

43	6	0	-2.657088	1.619633	-1.069436
44	6	0	-3.371582	0.520845	-3.527344
45	1	0	-1.350969	-0.176974	-3.641613
46	6	0	-3.956017	1.781012	-1.560192
47	1	0	-2.391356	2.073733	-0.121539
48	6	0	-4.320039	1.229459	-2.786705
49	1	0	-3.635776	0.099108	-4.492798
50	1	0	-4.680620	2.347902	-0.981984
51	1	0	-5.328425	1.357786	-3.168740

Equatorial conformation of **1b**x2HCHO:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.717196	-0.301619	-0.838471
2	1	0	-0.610003	-1.390804	-0.919765
3	6	0	0.717196	0.301619	-0.838471
4	1	0	0.610003	1.390804	-0.919765
5	6	0	2.624401	-0.009315	0.652911
6	6	0	-2.624401	0.009315	0.652911
7	1	0	3.242097	0.035398	-0.244821
8	1	0	-3.242097	-0.035398	-0.244821
9	7	0	-1.323254	-0.041421	0.499007
10	7	0	1.323254	0.041421	0.499007
11	24	0	0.000000	0.000000	2.001469
12	8	0	1.401890	0.001832	3.350187
13	8	0	-1.401890	-0.001832	3.350187
14	6	0	3.301675	-0.111222	1.895244
15	1	0	4.383084	-0.178029	1.874060
16	6	0	-3.301675	0.111222	1.895244
17	1	0	-4.383084	0.178029	1.874060
18	6	0	-2.677846	0.087108	3.125075
19	1	0	-3.296350	0.137691	4.026309
20	6	0	2.677846	-0.087108	3.125075
21	1	0	3.296350	-0.137691	4.026309
22	8	0	0.021382	-2.061095	2.046858
23	8	0	-0.021382	2.061095	2.046858
24	6	0	0.000000	2.723814	3.078246
25	6	0	0.000000	-2.723814	3.078246
26	1	0	-0.029668	-2.245372	4.064903
27	1	0	0.009943	-3.818912	3.011079
28	1	0	-0.009943	3.818912	3.011079
29	1	0	0.029668	2.245372	4.064903
30	6	0	-1.540674	0.188028	-2.016209
31	6	0	-1.986892	-0.718851	-2.984193
32	6	0	-1.857955	1.547511	-2.164134
33	6	0	-2.726023	-0.280129	-4.084710
34	1	0	-1.747238	-1.774584	-2.883071

35	6	0	-2.598574	1.986513	-3.260331
36	1	0	-1.535003	2.266899	-1.414948
37	6	0	-3.032424	1.073214	-4.225003
38	1	0	-3.061047	-0.996459	-4.829130
39	1	0	-2.837501	3.041244	-3.362686
40	1	0	-3.608171	1.416553	-5.079515
41	6	0	1.540674	-0.188028	-2.016209
42	6	0	1.986892	0.718851	-2.984193
43	6	0	1.857955	-1.547511	-2.164134
44	6	0	2.726023	0.280129	-4.084710
45	1	0	1.747238	1.774584	-2.883071
46	6	0	2.598574	-1.986513	-3.260331
47	1	0	1.535003	-2.266899	-1.414948
48	6	0	3.032424	-1.073214	-4.225003
49	1	0	3.061047	0.996459	-4.829130
50	1	0	2.837501	-3.041244	-3.362686
51	1	0	3.608171	-1.416553	-5.079515

Axial conformation of **1c**x2HCHO:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.353243	-0.689853	-2.318457
2	6	0	-0.353243	0.689853	-2.318457
3	6	0	-0.083401	2.602695	-0.860093
4	6	0	0.083401	-2.602695	-0.860093
5	1	0	-0.110925	3.200546	-1.775553
6	1	0	0.110925	-3.200546	-1.775553
7	7	0	0.146872	-1.299730	-0.984042
8	7	0	-0.146872	1.299730	-0.984042
9	24	0	0.000000	0.000000	0.536554
10	8	0	-0.130568	1.428618	1.853238
11	8	0	0.130568	-1.428618	1.853238
12	6	0	0.000000	3.306494	0.367682
13	1	0	0.065732	4.387306	0.329401
14	6	0	0.000000	-3.306494	0.367682
15	1	0	-0.065732	-4.387306	0.329401
16	6	0	0.050445	-2.701507	1.607689
17	1	0	0.033081	-3.335965	2.498756
18	6	0	-0.050445	2.701507	1.607689
19	1	0	-0.033081	3.335965	2.498756
20	8	0	2.048901	0.228809	0.632489
21	8	0	-2.048901	-0.228809	0.632489
22	6	0	-2.729329	-0.008442	1.628516
23	6	0	2.729329	0.008442	1.628516
24	1	0	2.281737	-0.389260	2.547741
25	1	0	3.807621	0.208206	1.593981
26	1	0	-3.807621	-0.208206	1.593981

27	1	0	-2.281737	0.389260	2.547741
28	1	0	-0.127616	-1.327256	-3.071785
29	1	0	0.127616	1.327256	-3.071785
30	6	0	1.848459	-0.581361	-2.648989
31	1	0	2.328331	-1.564195	-2.599089
32	1	0	1.980779	-0.193224	-3.664662
33	1	0	2.361849	0.088746	-1.953038
34	6	0	-1.848459	0.581361	-2.648989
35	1	0	-2.328331	1.564195	-2.599089
36	1	0	-1.980779	0.193224	-3.664662
37	1	0	-2.361849	-0.088746	-1.953038

Equatorial conformation of **1c**x2HCHO:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.685703	-0.364712	-2.208203
2	6	0	0.685703	0.364712	-2.208203
3	6	0	2.612140	-0.035537	-0.736932
4	6	0	-2.612140	0.035537	-0.736932
5	1	0	3.243859	-0.016445	-1.624119
6	1	0	-3.243859	0.016445	-1.624119
7	7	0	-1.317151	-0.091634	-0.890051
8	7	0	1.317151	0.091634	-0.890051
9	24	0	0.000000	0.000000	0.621429
10	8	0	1.402086	0.033453	1.966686
11	8	0	-1.402086	-0.033453	1.966686
12	6	0	3.286252	-0.179529	0.503985
13	1	0	4.362999	-0.298427	0.478115
14	6	0	-3.286252	0.179529	0.503985
15	1	0	-4.362999	0.298427	0.478115
16	6	0	-2.671824	0.112458	1.736778
17	1	0	-3.293307	0.175021	2.635020
18	6	0	2.671824	-0.112458	1.736778
19	1	0	3.293307	-0.175021	2.635020
20	8	0	0.082255	-2.057923	0.663016
21	8	0	-0.082255	2.057923	0.663016
22	6	0	0.000000	2.729931	1.685499
23	6	0	0.000000	-2.729931	1.685499
24	1	0	-0.134967	-2.261374	2.668225
25	1	0	0.059881	-3.823045	1.613254
26	1	0	-0.059881	3.823045	1.613254
27	1	0	0.134967	2.261374	2.668225
28	1	0	0.473730	1.444198	-2.231388
29	1	0	-0.473730	-1.444198	-2.231388
30	6	0	1.555363	0.008399	-3.414869
31	1	0	1.027820	0.237572	-4.343138
32	1	0	2.477770	0.595669	-3.435965

33	1	0	1.818024	-1.055776	-3.421963
34	6	0	-1.555363	-0.008399	-3.414869
35	1	0	-2.477770	-0.595669	-3.435965
36	1	0	-1.818024	1.055776	-3.421963
37	1	0	-1.027820	-0.237572	-4.343138

Axial conformation of **1d**x2HCHO:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.552340	-0.548014	-1.149222
2	6	0	0.552340	0.548014	-1.149222
3	6	0	2.499370	0.652243	0.296698
4	6	0	-2.499370	-0.652243	0.296698
5	1	0	3.079808	0.785261	-0.619909
6	1	0	-3.079808	-0.785261	-0.619909
7	7	0	-1.206471	-0.479062	0.177752
8	7	0	1.206471	0.479062	0.177752
9	24	0	0.000000	0.000000	1.702976
10	8	0	1.348951	0.500203	3.019008
11	8	0	-1.348951	-0.500203	3.019008
12	6	0	3.210949	0.708289	1.523399
13	1	0	4.284462	0.848793	1.478836
14	6	0	-3.210949	-0.708289	1.523399
15	1	0	-4.284462	-0.848793	1.478836
16	6	0	-2.612800	-0.666978	2.766193
17	1	0	-3.241215	-0.795127	3.652563
18	6	0	2.612800	0.666978	2.766193
19	1	0	3.241215	0.795127	3.652563
20	8	0	0.761143	-1.916357	1.808478
21	8	0	-0.761143	1.916357	1.808478
22	6	0	-0.696602	2.635252	2.799510
23	6	0	0.696602	-2.635252	2.799510
24	1	0	0.160463	-2.314771	3.701409
25	1	0	1.179669	-3.620208	2.777402
26	1	0	-1.179669	3.620208	2.777402
27	1	0	-0.160463	2.314771	3.701409
28	1	0	-1.306043	-0.307748	-1.908297
29	1	0	1.306043	0.307748	-1.908297
30	6	0	-0.005683	1.965734	-1.479264
31	6	0	0.999601	3.094988	-1.175492
32	6	0	-0.430784	2.047040	-2.963911
33	1	0	-0.895902	2.131093	-0.855199
34	6	0	0.441245	4.480717	-1.540964
35	1	0	1.924314	2.919923	-1.747775
36	1	0	1.282729	3.083804	-0.116885
37	6	0	-0.995030	3.428844	-3.332010
38	1	0	0.446682	1.836805	-3.594296

39	1	0	-1.174454	1.278626	-3.206511
40	6	0	0.000000	4.549837	-3.008063
41	1	0	1.195912	5.247977	-1.330254
42	1	0	-0.419824	4.703454	-0.893052
43	1	0	-1.257769	3.444587	-4.396324
44	1	0	-1.930081	3.598038	-2.778156
45	1	0	-0.443197	5.528409	-3.226709
46	1	0	0.881602	4.453013	-3.657952
47	6	0	0.005683	-1.965734	-1.479264
48	6	0	-0.999601	-3.094988	-1.175492
49	6	0	0.430784	-2.047040	-2.963911
50	1	0	0.895902	-2.131093	-0.855199
51	6	0	-0.441245	-4.480717	-1.540964
52	1	0	-1.924314	-2.919923	-1.747775
53	1	0	-1.282729	-3.083804	-0.116885
54	6	0	0.995030	-3.428844	-3.332010
55	1	0	-0.446682	-1.836805	-3.594296
56	1	0	1.174454	-1.278626	-3.206511
57	6	0	0.000000	-4.549837	-3.008063
58	1	0	-1.195912	-5.247977	-1.330254
59	1	0	0.419824	-4.703454	-0.893052
60	1	0	1.257769	-3.444587	-4.396324
61	1	0	1.930081	-3.598038	-2.778156
62	1	0	0.443197	-5.528409	-3.226709
63	1	0	-0.881602	-4.453013	-3.657952

Equatorial conformation of **1d**x2HCHO:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.685058	0.384469	-0.676372
2	1	0	0.436255	1.451883	-0.589092
3	6	0	-0.685058	-0.384469	-0.676372
4	1	0	-0.436255	-1.451883	-0.589092
5	6	0	-2.593082	0.220551	0.792332
6	6	0	2.593082	-0.220551	0.792332
7	1	0	-3.233772	0.254492	-0.082035
8	1	0	3.233772	-0.254492	-0.082035
9	7	0	1.320225	0.033225	0.626098
10	7	0	-1.320225	-0.033225	0.626098
11	24	0	0.000000	0.000000	2.140803
12	8	0	-1.394372	0.015145	3.496499
13	8	0	1.394372	-0.015145	3.496499
14	6	0	-3.243116	0.437187	2.038541
15	1	0	-4.302648	0.663452	2.013153
16	6	0	3.243116	-0.437187	2.038541
17	1	0	4.302648	-0.663452	2.013153
18	6	0	2.643651	-0.291207	3.269883

19	1	0	3.258177	-0.399251	4.168683
20	6	0	-2.643651	0.291207	3.269883
21	1	0	-3.258177	0.399251	4.168683
22	8	0	0.000000	2.060409	2.186723
23	8	0	0.000000	-2.060409	2.186723
24	6	0	-0.198607	-2.722402	3.199523
25	6	0	0.198607	2.722402	3.199523
26	1	0	0.415788	2.241852	4.161416
27	1	0	0.163308	3.817329	3.138049
28	1	0	-0.163308	-3.817329	3.138049
29	1	0	-0.415788	-2.241852	4.161416
30	6	0	-1.521958	-0.246054	-1.976583
31	6	0	-2.649775	-1.298551	-2.123479
32	6	0	-2.006596	1.176186	-2.339388
33	1	0	-0.810788	-0.526937	-2.764452
34	6	0	-3.257776	-1.250464	-3.535360
35	1	0	-3.455487	-1.146040	-1.395919
36	1	0	-2.242250	-2.298206	-1.921213
37	6	0	-2.634329	1.199596	-3.744801
38	1	0	-2.747253	1.540521	-1.616355
39	1	0	-1.170775	1.886550	-2.296877
40	6	0	-3.754762	0.159520	-3.886668
41	1	0	-4.076919	-1.975235	-3.609803
42	1	0	-2.498720	-1.561401	-4.267799
43	1	0	-3.014436	2.204686	-3.962106
44	1	0	-1.853372	0.993907	-4.491431
45	1	0	-4.155707	0.175351	-4.906739
46	1	0	-4.588708	0.428639	-3.221344
47	6	0	1.521958	0.246054	-1.976583
48	6	0	2.649775	1.298551	-2.123479
49	6	0	2.006596	-1.176186	-2.339388
50	1	0	0.810788	0.526937	-2.764452
51	6	0	3.257776	1.250464	-3.535360
52	1	0	3.455487	1.146040	-1.395919
53	1	0	2.242250	2.298206	-1.921213
54	6	0	2.634329	-1.199596	-3.744801
55	1	0	2.747253	-1.540521	-1.616355
56	1	0	1.170775	-1.886550	-2.296877
57	6	0	3.754762	-0.159520	-3.886668
58	1	0	4.076919	1.975235	-3.609803
59	1	0	2.498720	1.561401	-4.267799
60	1	0	3.014436	-2.204686	-3.962106
61	1	0	1.853372	-0.993907	-4.491431
62	1	0	4.155707	-0.175351	-4.906739
63	1	0	4.588708	-0.428639	-3.221344

Axial conformation of **1e**x2HCHO:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.761471	0.176989	-1.609949
2	6	0	-0.761471	-0.176989	-1.609949
3	6	0	-2.521819	0.477436	-0.087284
4	6	0	2.521819	-0.477436	-0.087284
5	1	0	-3.097097	0.684007	-0.992111
6	1	0	3.097097	-0.684007	-0.992111
7	7	0	1.289187	-0.049836	-0.236221
8	7	0	-1.289187	0.049836	-0.236221
9	24	0	0.000000	0.000000	1.302730
10	8	0	-1.435033	0.029806	2.629484
11	8	0	1.435033	-0.029806	2.629484
12	6	0	-3.196894	0.675723	1.144106
13	1	0	-4.226745	1.010299	1.102513
14	6	0	3.196894	-0.675723	1.144106
15	1	0	4.226745	-1.010299	1.102513
16	6	0	2.652869	-0.406029	2.383033
17	1	0	3.288511	-0.507165	3.267799
18	6	0	-2.652869	0.406029	2.383033
19	1	0	-3.288511	0.507165	3.267799
20	8	0	0.000000	2.057154	1.512705
21	8	0	0.000000	-2.057154	1.512705
22	6	0	-0.313591	-2.651993	2.537791
23	6	0	0.313591	2.651993	2.537791
24	1	0	0.694962	2.114669	3.414486
25	1	0	0.216825	3.744647	2.569910
26	1	0	-0.216825	-3.744647	2.569910
27	1	0	-0.694962	-2.114669	3.414486
28	1	0	1.280725	-0.532979	-2.262591
29	1	0	-1.280725	0.532979	-2.262591
30	6	0	1.101485	1.601099	-2.218746
31	6	0	-1.101485	-1.601099	-2.218746
32	6	0	-0.292345	-2.755170	-1.600859
33	1	0	-0.535561	-3.688098	-2.121496
34	1	0	0.788989	-2.608243	-1.694945
35	1	0	-0.521079	-2.897673	-0.543761
36	6	0	0.292345	2.755170	-1.600859
37	1	0	0.535561	3.688098	-2.121496
38	1	0	-0.788989	2.608243	-1.694945
39	1	0	0.521079	2.897673	-0.543761
40	6	0	-2.602506	-1.909090	-2.048389
41	1	0	-3.234781	-1.142247	-2.512851
42	1	0	-2.838750	-2.858871	-2.539772
43	1	0	-2.893487	-2.005496	-0.997502
44	6	0	2.602506	1.909090	-2.048389
45	1	0	3.234781	1.142247	-2.512851
46	1	0	2.838750	2.858871	-2.539772
47	1	0	2.893487	2.005496	-0.997502
48	6	0	0.810150	1.556058	-3.736055

49	1	0	1.097110	2.509839	-4.191300
50	1	0	1.381737	0.767008	-4.237791
51	1	0	-0.249932	1.399799	-3.959213
52	6	0	-0.810150	-1.556058	-3.736055
53	1	0	-1.097110	-2.509839	-4.191300
54	1	0	-1.381737	-0.767008	-4.237791
55	1	0	0.249932	-1.399799	-3.959213

Equatorial conformation of **1e**x2HCHO:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.458956	0.662191	-1.282010
2	1	0	-1.462294	0.289174	-1.044264
3	6	0	0.458956	-0.662191	-1.282010
4	1	0	1.462294	-0.289174	-1.044264
5	6	0	-0.557031	-2.479356	0.106832
6	6	0	0.557031	2.479356	0.106832
7	1	0	-0.743296	-3.063206	-0.789463
8	1	0	0.743296	3.063206	-0.789463
9	7	0	0.000000	1.300408	-0.005991
10	7	0	0.000000	-1.300408	-0.005991
11	24	0	0.000000	0.000000	1.522151
12	8	0	-0.117639	-1.425909	2.845946
13	8	0	0.117639	1.425909	2.845946
14	6	0	-0.914539	-3.102895	1.334994
15	1	0	-1.355350	-4.091476	1.280367
16	6	0	0.914539	3.102895	1.334994
17	1	0	1.355350	4.091476	1.280367
18	6	0	0.626806	2.592676	2.583403
19	1	0	0.824360	3.214359	3.461836
20	6	0	-0.626806	-2.592676	2.583403
21	1	0	-0.824360	-3.214359	3.461836
22	8	0	-2.059654	0.121298	1.583097
23	8	0	2.059654	-0.121298	1.583097
24	6	0	2.697903	-0.523751	2.549674
25	6	0	-2.697903	0.523751	2.549674
26	1	0	-2.192240	0.888672	3.452457
27	1	0	-3.794182	0.524013	2.503822
28	1	0	3.794182	-0.524013	2.503822
29	1	0	2.192240	-0.888672	3.452457
30	6	0	0.719759	-1.637612	-2.488364
31	6	0	1.708026	-2.740076	-2.009584
32	6	0	-0.549448	-2.301931	-3.100332
33	1	0	1.301854	-3.410175	-1.249475
34	1	0	2.627084	-2.297288	-1.607407
35	1	0	-0.647878	-3.350174	-2.797963

36	1	0	-1.476669	-1.792939	-2.825299
37	6	0	-0.719759	1.637612	-2.488364
38	6	0	-1.708026	2.740076	-2.009584
39	6	0	0.549448	2.301931	-3.100332
40	1	0	-1.301854	3.410175	-1.249475
41	1	0	-2.627084	2.297288	-1.607407
42	1	0	0.647878	3.350174	-2.797963
43	1	0	1.476669	1.792939	-2.825299
44	1	0	-1.991787	3.360839	-2.865940
45	1	0	0.496512	2.305651	-4.193815
46	1	0	-0.496512	-2.305651	-4.193815
47	1	0	1.991787	-3.360839	-2.865940
48	6	0	1.512538	-0.887244	-3.587653
49	1	0	2.420043	-0.427319	-3.178853
50	1	0	1.828573	-1.606808	-4.350023
51	1	0	0.942368	-0.111474	-4.093958
52	6	0	-1.512538	0.887244	-3.587653
53	1	0	-0.942368	0.111474	-4.093958
54	1	0	-2.420043	0.427319	-3.178853
55	1	0	-1.828573	1.606808	-4.350023

3.6 Coordinates of transition states optimized at B3LYP/6-31G(d).

Ts1:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.884867	0.573241	2.319721
2	1	0	-2.707389	1.249325	2.051286
3	6	0	-0.572660	1.366441	2.362870
4	1	0	0.201061	0.764152	2.855549
5	6	0	0.287471	2.785813	0.593869
6	6	0	-2.444831	-1.570927	1.361338
7	1	0	0.312187	3.596325	1.328905
8	1	0	-3.042962	-1.741947	2.261340
9	7	0	-1.761899	-0.459900	1.283258
10	7	0	-0.156087	1.619608	0.981314
11	24	0	-0.514089	0.041618	-0.229441
12	8	0	0.565055	0.874461	-1.658038
13	8	0	-1.156088	-1.462193	-1.309743
14	6	0	0.763931	3.073804	-0.712687
15	1	0	1.085340	4.086898	-0.924201
16	6	0	-2.495300	-2.565895	0.350722
17	1	0	-3.085737	-3.453921	0.543239
18	6	0	-1.896278	-2.441603	-0.886808
19	1	0	-2.053815	-3.241296	-1.617861
20	6	0	0.885044	2.129841	-1.716692

21	1	0	1.317047	2.447836	-2.671636
22	8	0	-2.146003	1.155903	-1.034764
23	8	0	0.965837	-0.980265	0.516803
24	6	0	1.490532	-2.070998	-0.052654
25	6	0	-2.612391	0.998551	-2.154627
26	1	0	-2.221820	0.227929	-2.832356
27	1	0	-3.442440	1.634724	-2.490461
28	1	0	1.775738	-2.840122	0.673653
29	1	0	0.886422	-2.497144	-0.861616
30	1	0	-2.111283	0.133292	3.298552
31	1	0	-0.695286	2.300112	2.925413
32	6	0	2.900919	-1.717004	-0.972401
33	1	0	3.068507	-2.574703	-1.623687
34	1	0	2.568300	-0.843458	-1.532911
35	6	0	3.155898	0.639414	0.772476
36	1	0	2.513188	0.790276	-0.081908
37	1	0	3.126067	1.401014	1.546078
38	6	0	3.928458	-1.521245	-0.001707
39	1	0	4.582290	-2.366621	0.211340
40	6	0	4.017023	-0.416850	0.867808
41	1	0	4.720496	-0.468197	1.694412

Ts2:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.024201	1.723269	2.149815
2	1	0	1.975362	2.234210	1.950556
3	6	0	1.303920	0.276956	2.568818
4	1	0	0.396818	-0.166190	2.999439
5	6	0	2.564412	-1.421916	1.388007
6	6	0	-0.394590	2.781296	0.515952
7	1	0	3.118644	-1.579654	2.317936
8	1	0	-0.406360	3.639859	1.194740
9	7	0	0.230294	1.701487	0.909166
10	7	0	1.661118	-0.479895	1.366645
11	24	0	0.530081	0.040888	-0.215663
12	8	0	1.201980	-1.483079	-1.248528
13	8	0	-0.513705	0.809658	-1.701981
14	6	0	2.869687	-2.271508	0.291954
15	1	0	3.661829	-2.999862	0.419300
16	6	0	-1.047145	2.940932	-0.733826
17	1	0	-1.542246	3.885028	-0.929584
18	6	0	-1.047582	1.987844	-1.737676
19	1	0	-1.557974	2.231379	-2.676027
20	6	0	2.179569	-2.265599	-0.903721
21	1	0	2.462931	-2.999581	-1.665045
22	8	0	2.205246	1.103561	-0.999002

23	8	0	-0.976224	-0.951446	0.526495
24	6	0	-1.445654	-2.067774	-0.016808
25	6	0	2.607857	1.015818	-2.150701
26	1	0	2.132605	0.338536	-2.872550
27	1	0	3.464263	1.622806	-2.473849
28	1	0	-1.735670	-2.829406	0.715003
29	1	0	-0.833032	-2.490113	-0.822083
30	1	0	0.505037	2.269866	2.946631
31	1	0	2.098669	0.234243	3.323416
32	6	0	-2.884651	-1.763045	-0.989700
33	1	0	-2.980397	-2.621423	-1.653473
34	1	0	-2.564557	-0.865627	-1.515657
35	6	0	-3.361109	0.573936	0.794666
36	1	0	-3.444232	1.335579	1.564638
37	1	0	-2.675165	0.778585	-0.014568
38	6	0	-3.919618	-1.648014	-0.027514
39	1	0	-4.508570	-2.542694	0.173933
40	6	0	-4.119463	-0.555851	0.850403
41	1	0	-4.847154	-0.675616	1.648575
