

Electronic Supplementary Information

Non-pericyclic Cycloaddition of *gem*-Difluorosubstituted Azomethine Ylides to the C=O Bond: Computational Study and Synthesis of Fluorinated Oxazole Derivatives

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Competition Experiments

Competition experiments for the reaction of aldehydes **3a-e** were performed as follows. A round bottom flask containing freshly prepared lead filings (0.3 mmol) and dry dichloromethane (5 mL) was charged with Bu₄NBr (0.6 mmol), *N*-benzhydrylidene-*N*-methylamine **11** (0.15-0.25 mmol), the competing pair of aldehydes (1-2.5 mmol in 1:1-2.5 mol ratio), CF₂Br₂ (0.6 mmol), and 2-methylnaphthalene (the internal standard). The flask was tightly stoppered, immersed into the thermostat bath and the reaction mixture was vigorously stirred by magnetic stirrer at 40 °C. After the reaction started, as evidenced by clouding of the solution, small samples were periodically removed for ¹H NMR analysis. While the aldehydes **3a-e** covered a wide range of σ values, to guarantee no aldehyde would react exclusively in the competition experiments, pairs of aldehydes were selected that were close in reactivity (Table 1). Relative constants were calculated using $k_1/k_2 = [H_1] \cdot [A_2]/[H_2] \cdot [A_1]$ for experiments where the conversion of the starting aldehydes was less than 10%. The [H_i] data were obtained via integration of the 5-H singlet of the product, and [A_i] data were obtained via integration of the aldehyde proton before the reaction started.

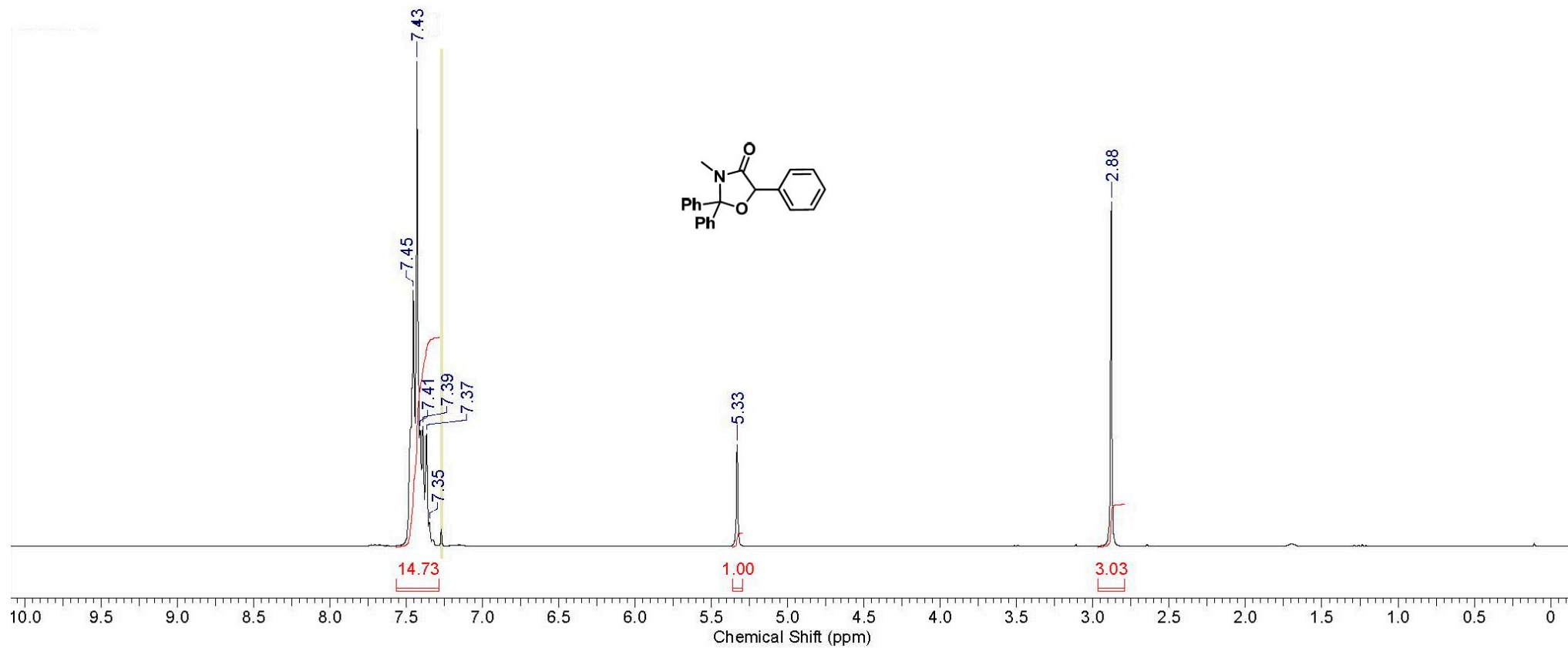
Table 1. Pairs of competing aldehydes **3a-e** and relative rate data for the reaction with azomethine ylide **12**.

Aldehyde N1/N2	n ^a	k ₁ /k ₂	s ^b	s _m ^c
3d/3c	6	9.49	1.24	0.51
3e/3d	11	3.39	0.41	0.12
3c/3a]	5	0.235	0.007	0.003
3b/3a	4	0.481	0.058	0.029

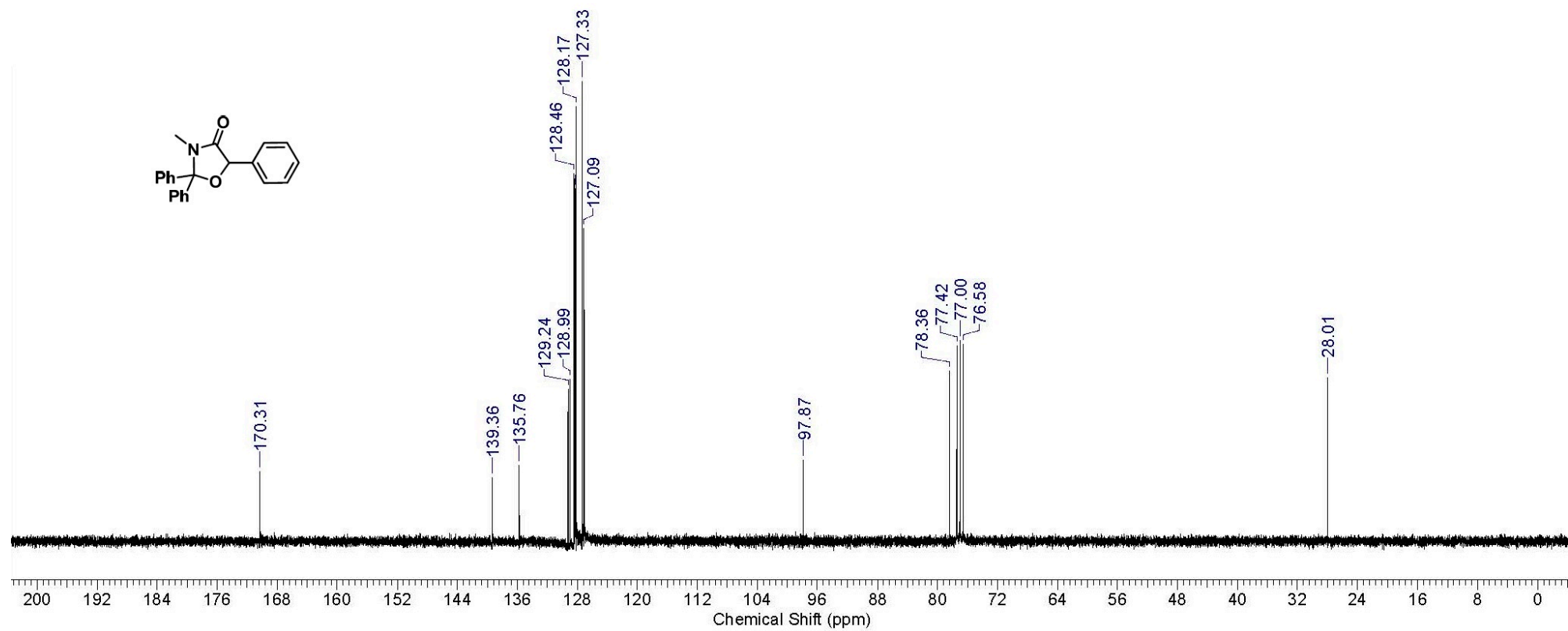
^a Number of experiments. ^b Standard deviation. ^c Standard mean square error.

NMR spectra

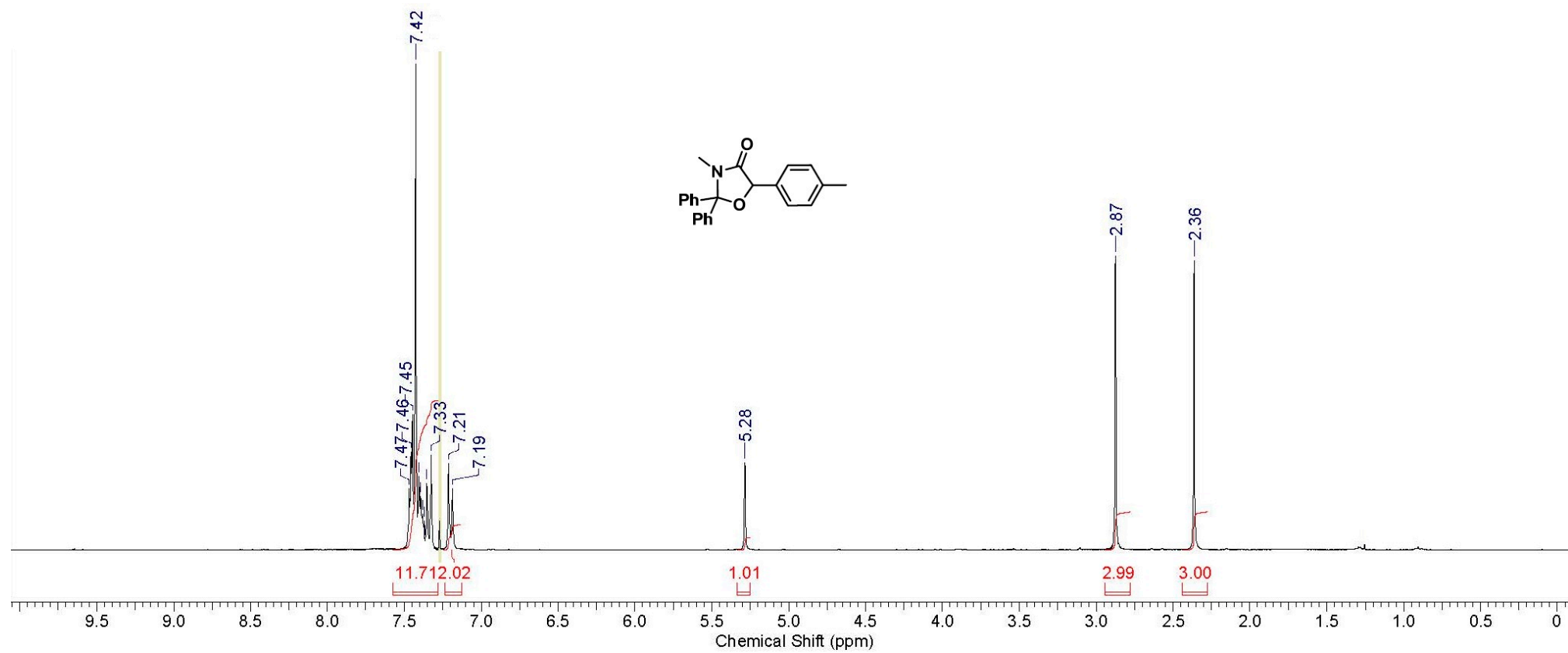
3-Methyl-2,2,5-triphenyloxazolidine-4-one (14a), 300(¹H) MHz, CDCl₃



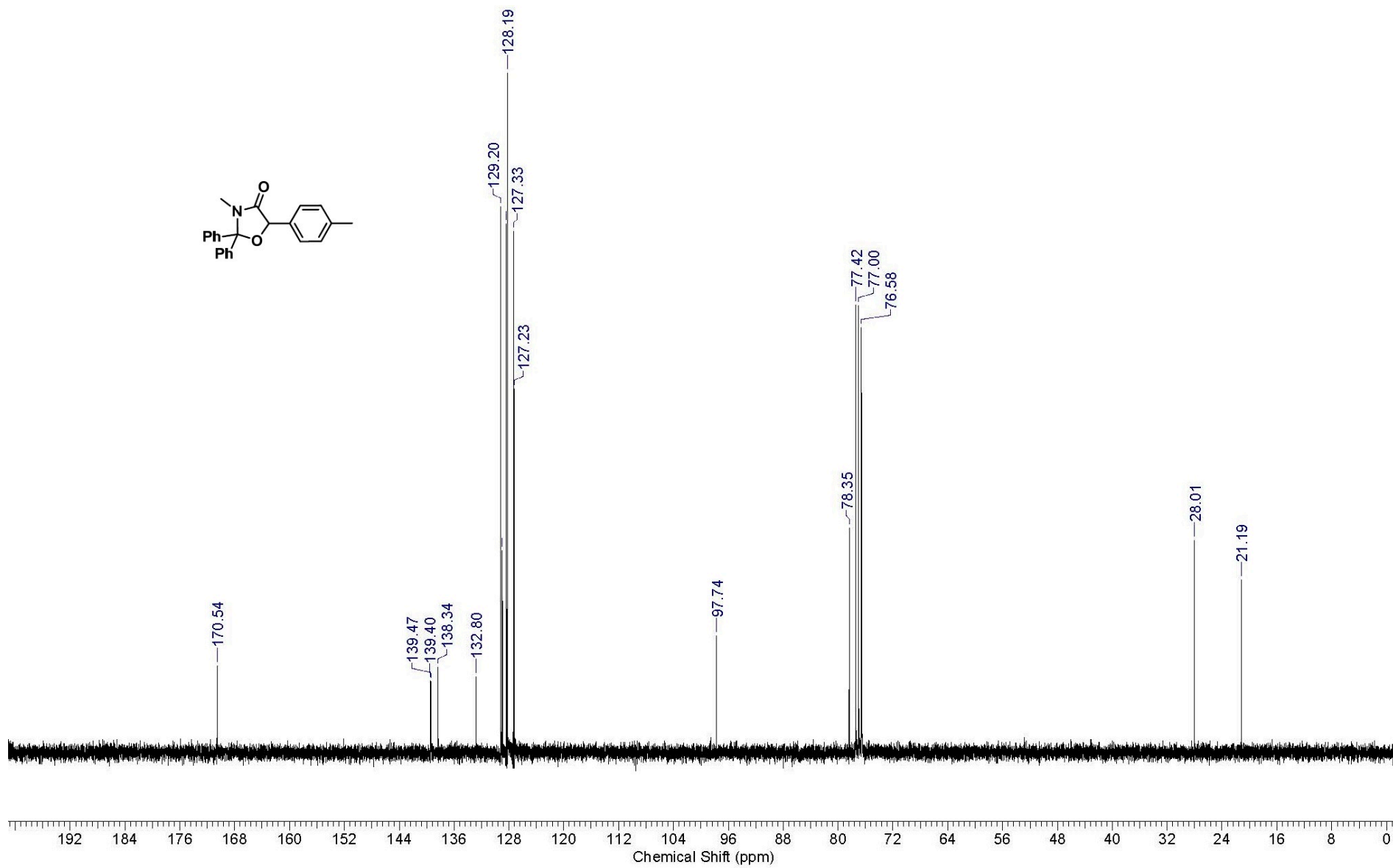
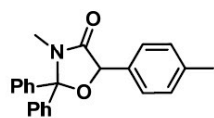
3-Methyl-2,2,5-triphenyloxazolidine-4-one (14a), 75(¹³C) MHz, CDCl₃



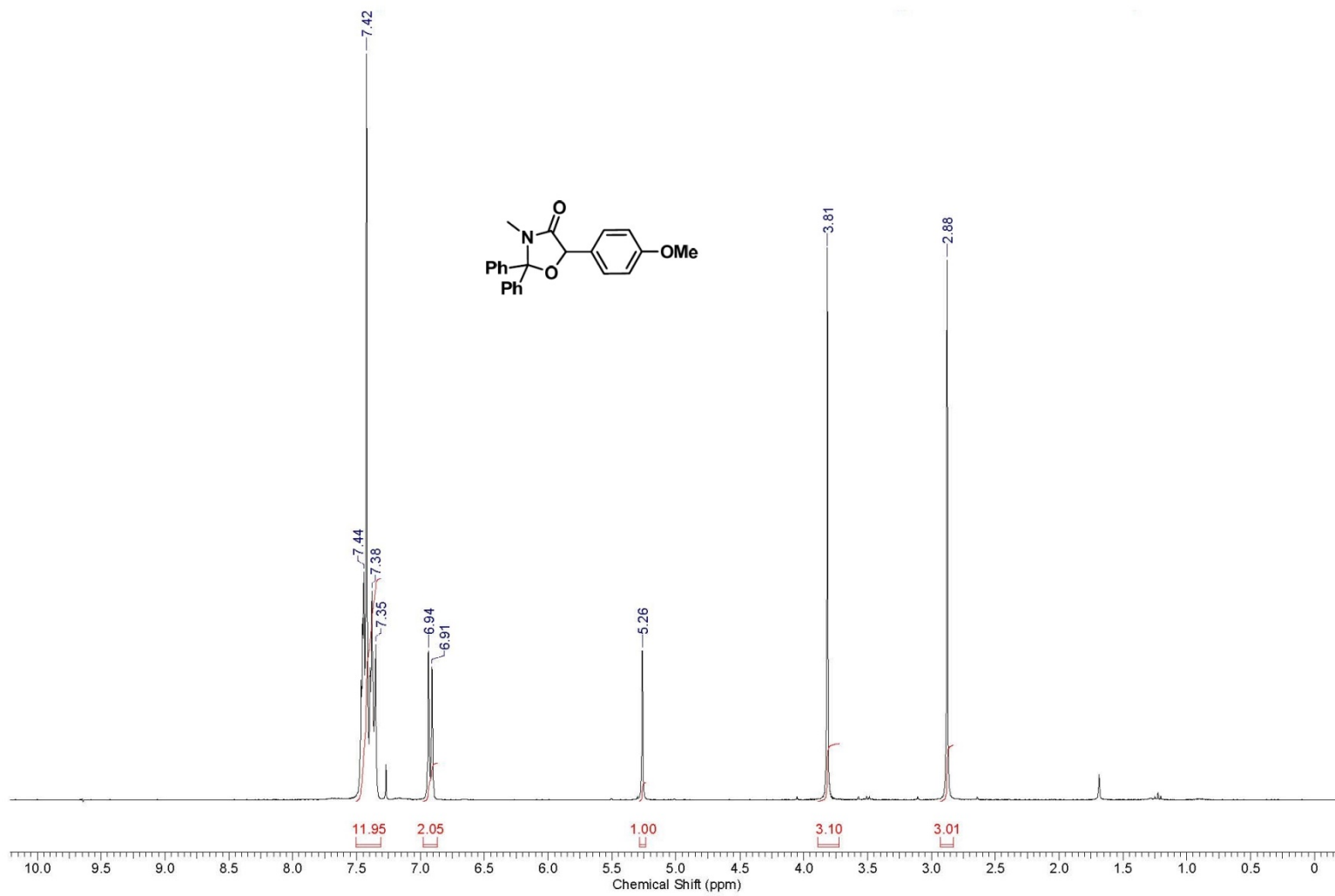
3-Methyl-2,2-diphenyl-5-(p-tolyl)oxazolidin-4-one (14b), 300(¹H) MHz, CDCl₃



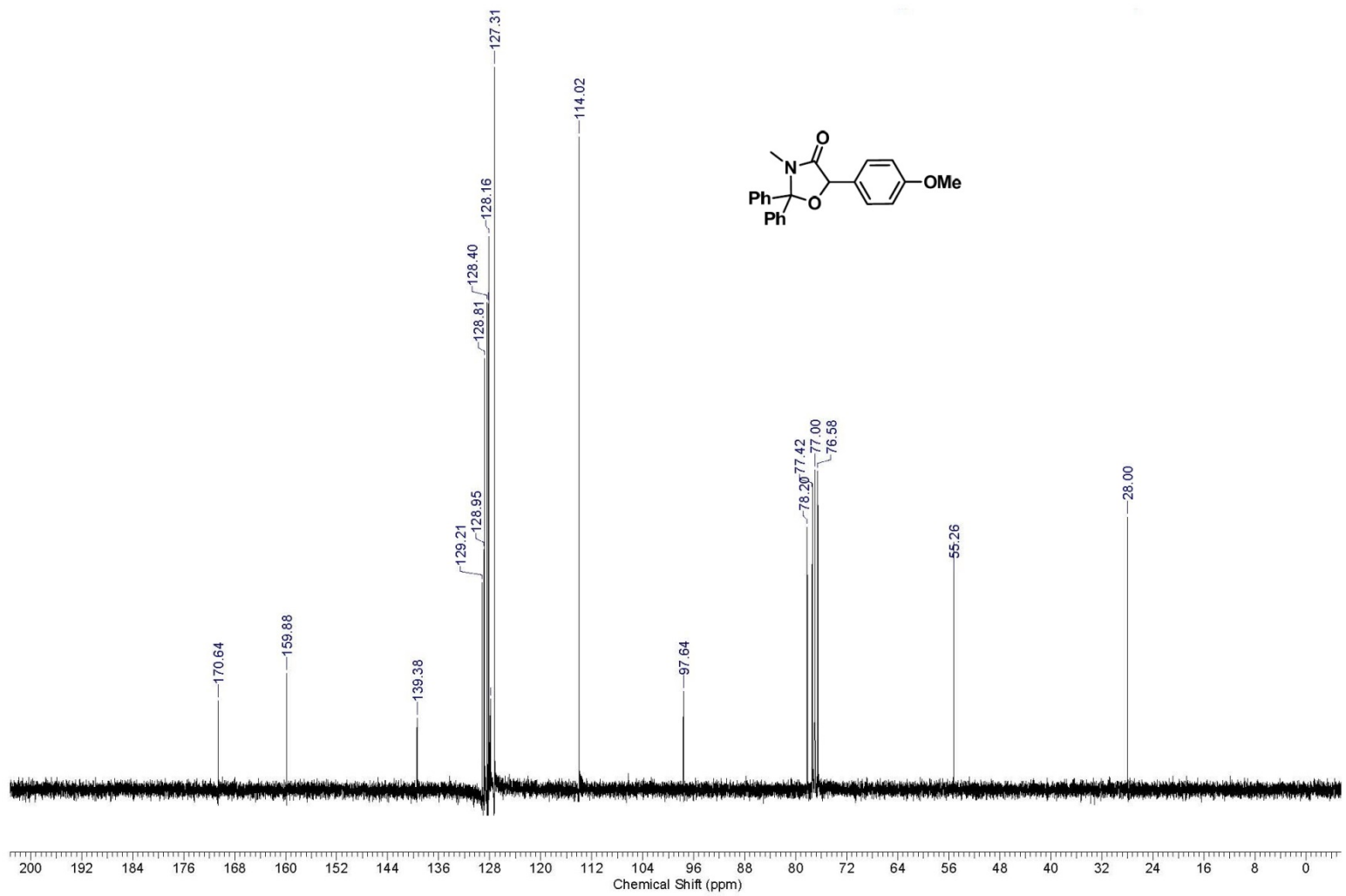
3-Methyl-2,2-diphenyl-5-(p-tolyl)oxazolidin-4-one (14b), 75(¹³C) MHz, CDCl₃



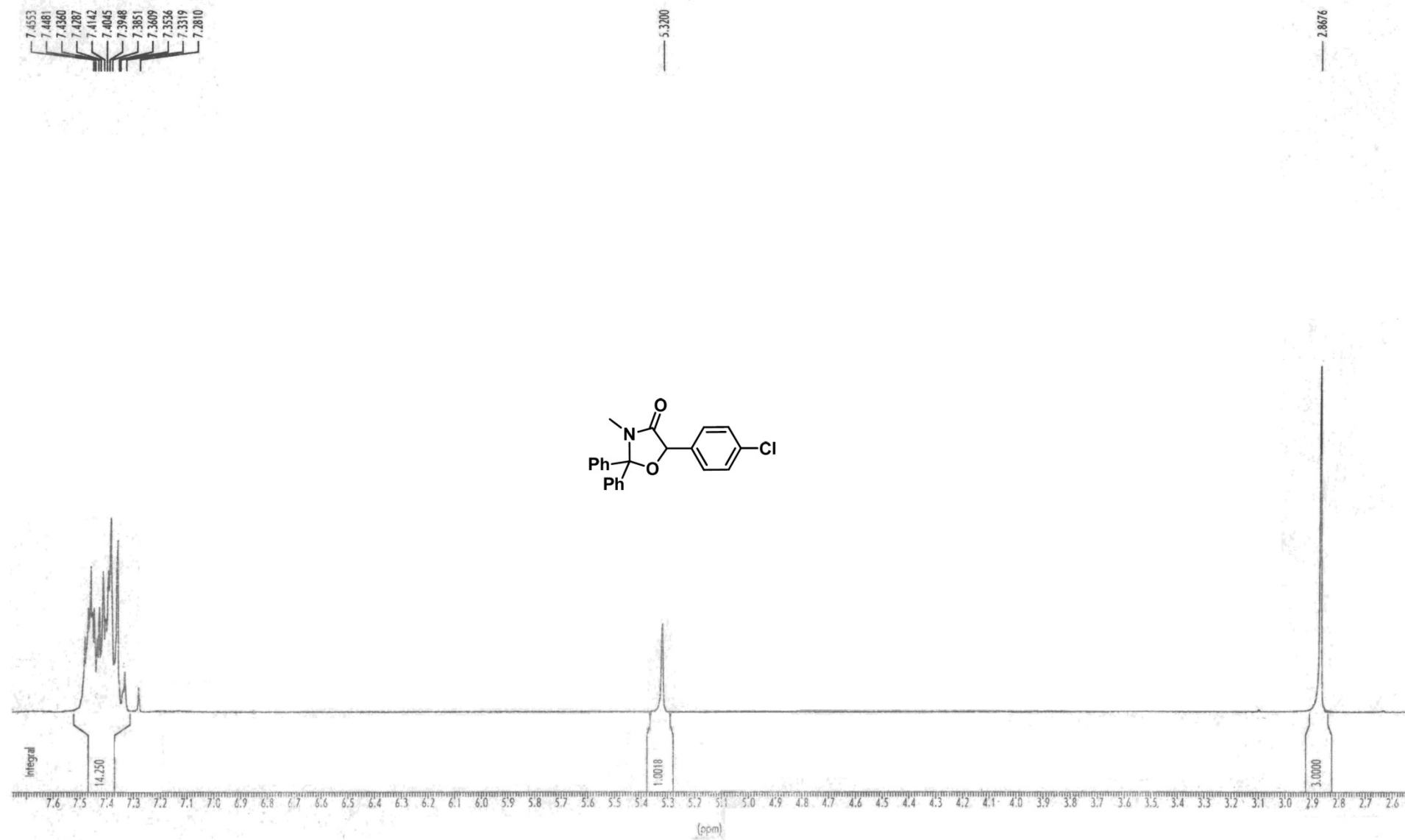
5-(4-Methoxyphenyl)-3-methyl-2,2-diphenyloxazolidin-4-one (14c), 300(¹H) MHz, CDCl₃



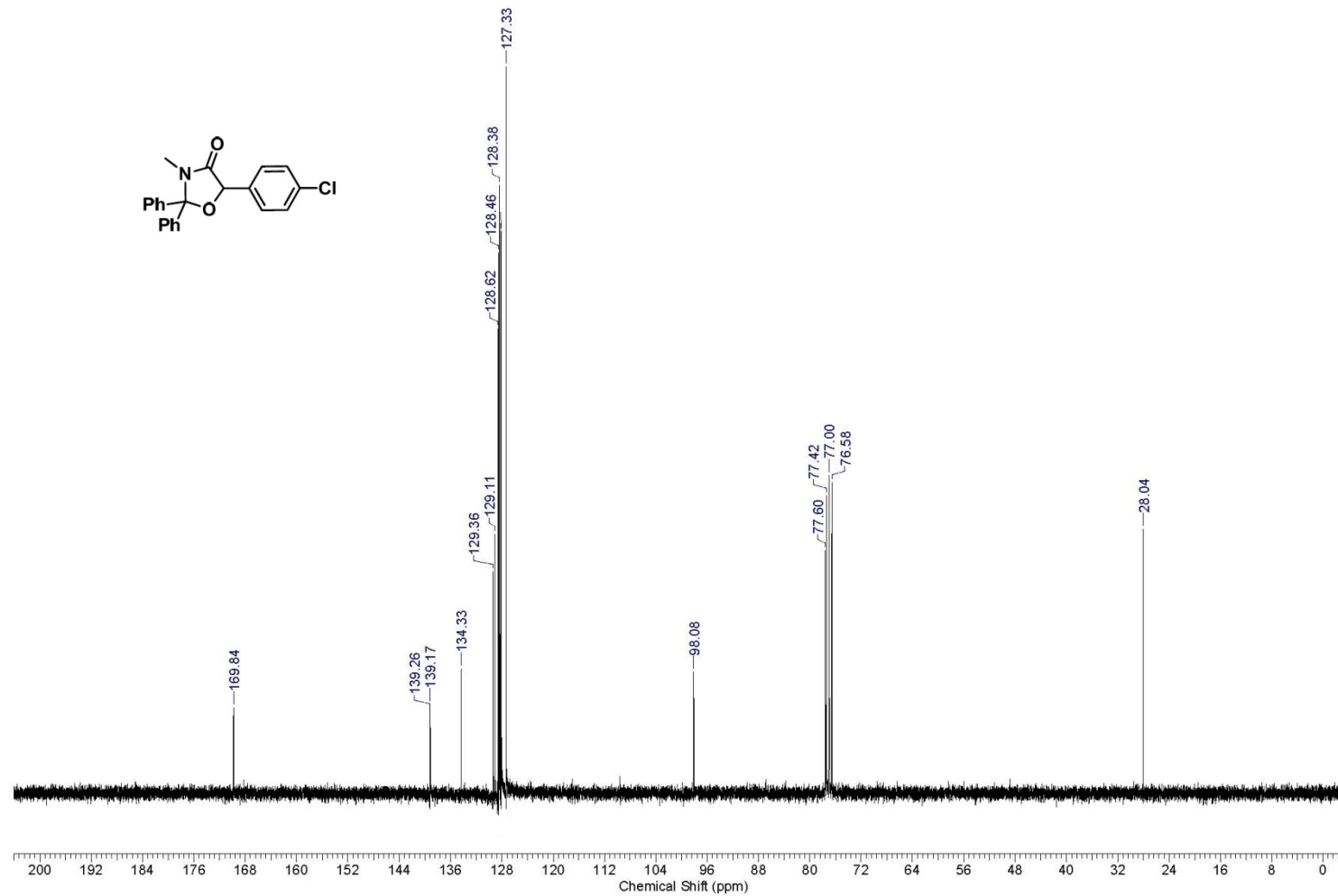
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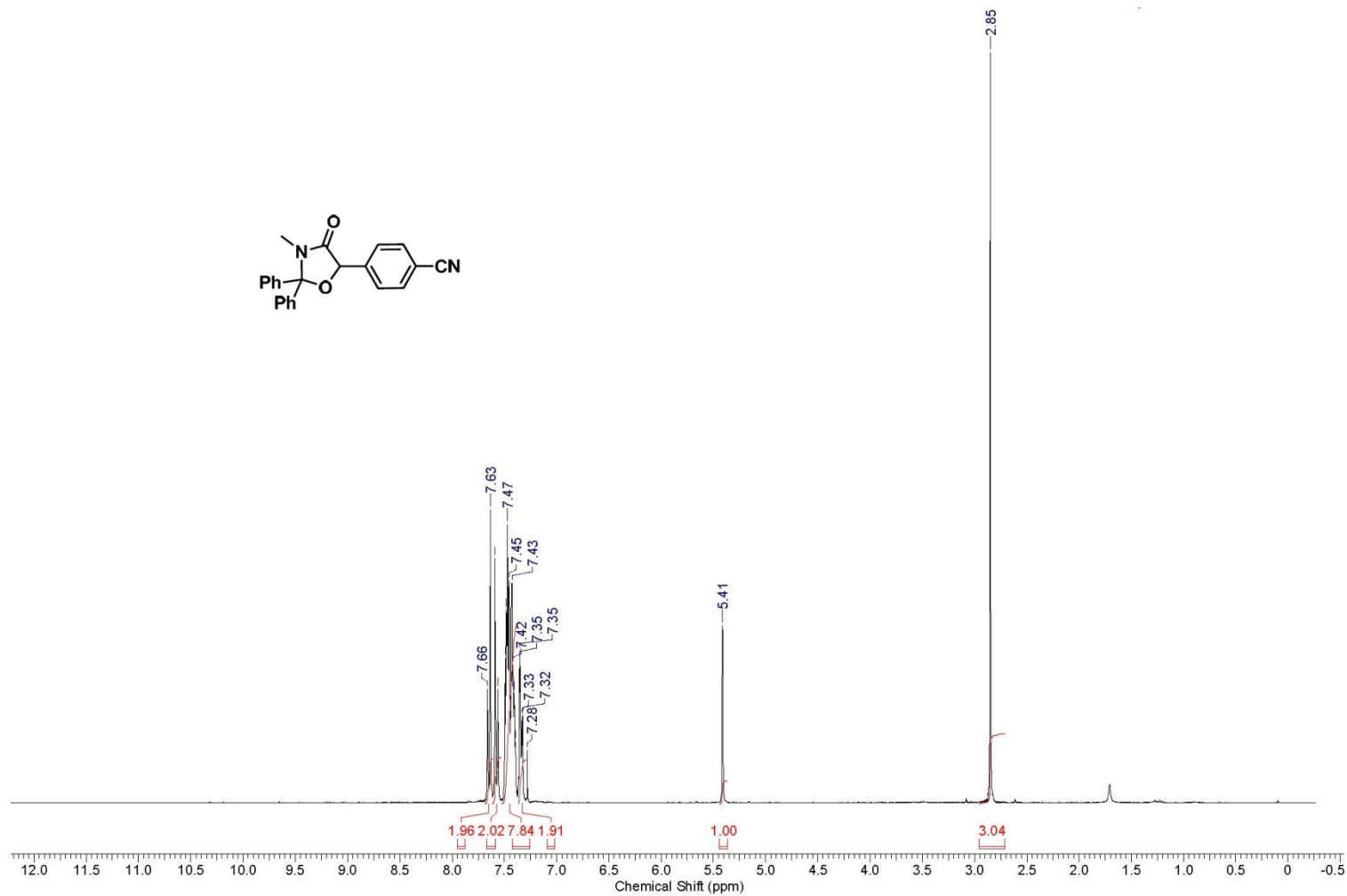
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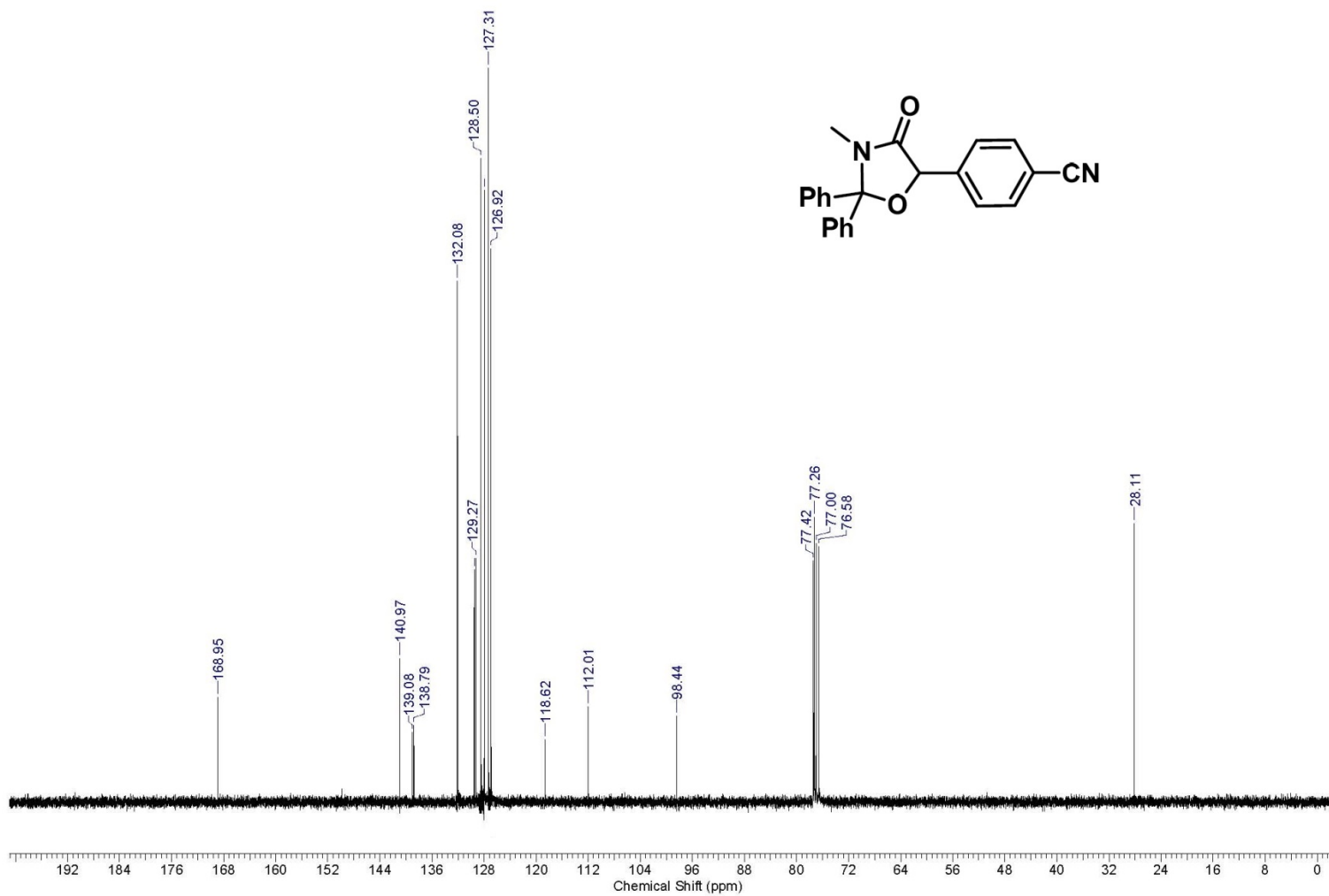
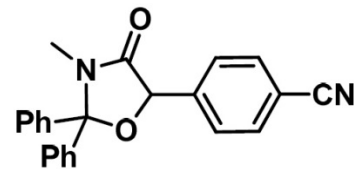
5-(4-Chlorophenyl)-3-methyl-2,2-diphenyloxazolidin-4-one (14d), 75(¹³C) MHz, CDCl₃



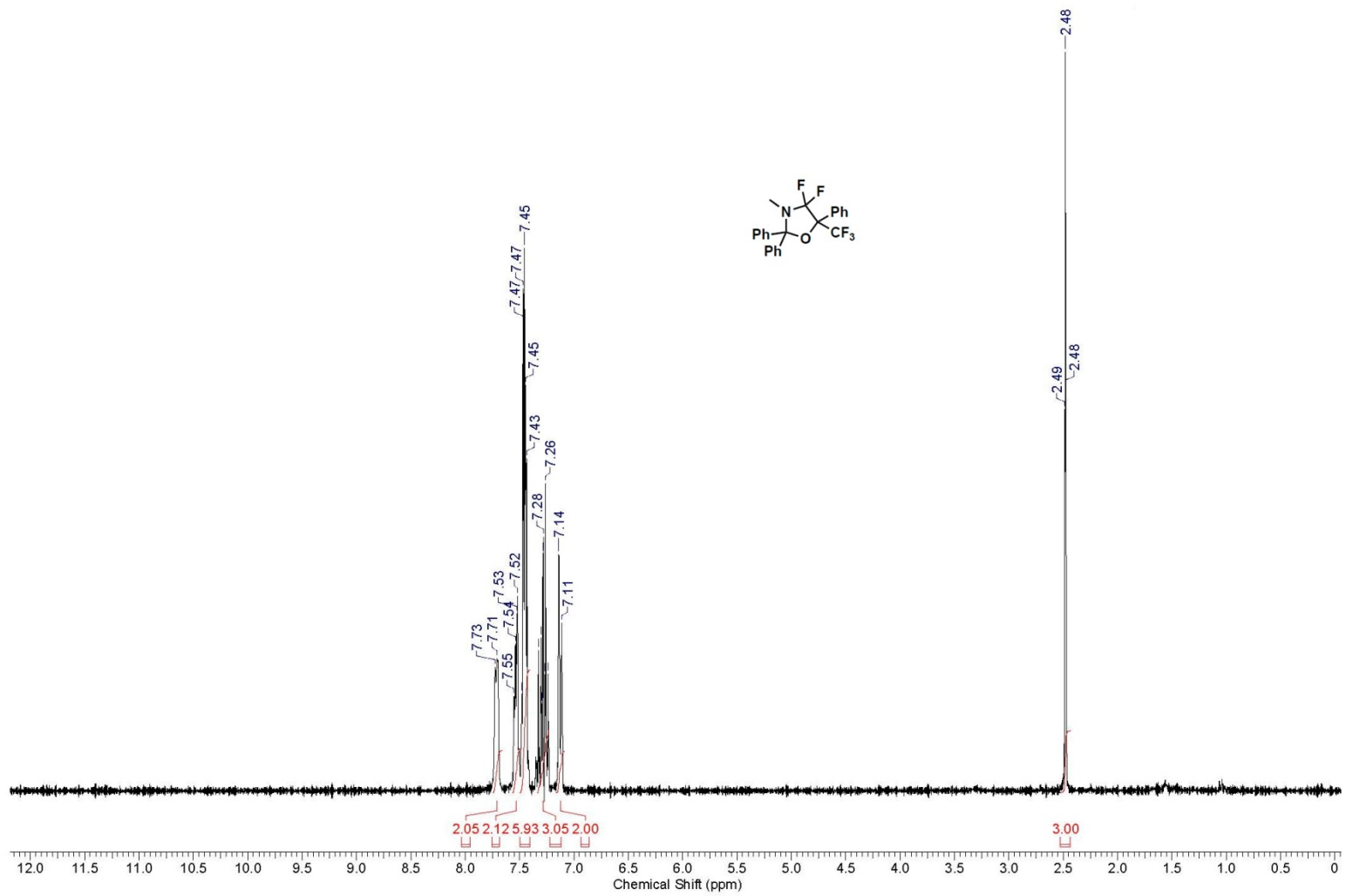
4-(3-Methyl-4-oxo-2,2-diphenyloxazolidin-5-yl)benzonitrile (14e), 300(¹H) MHz, CDCl₃



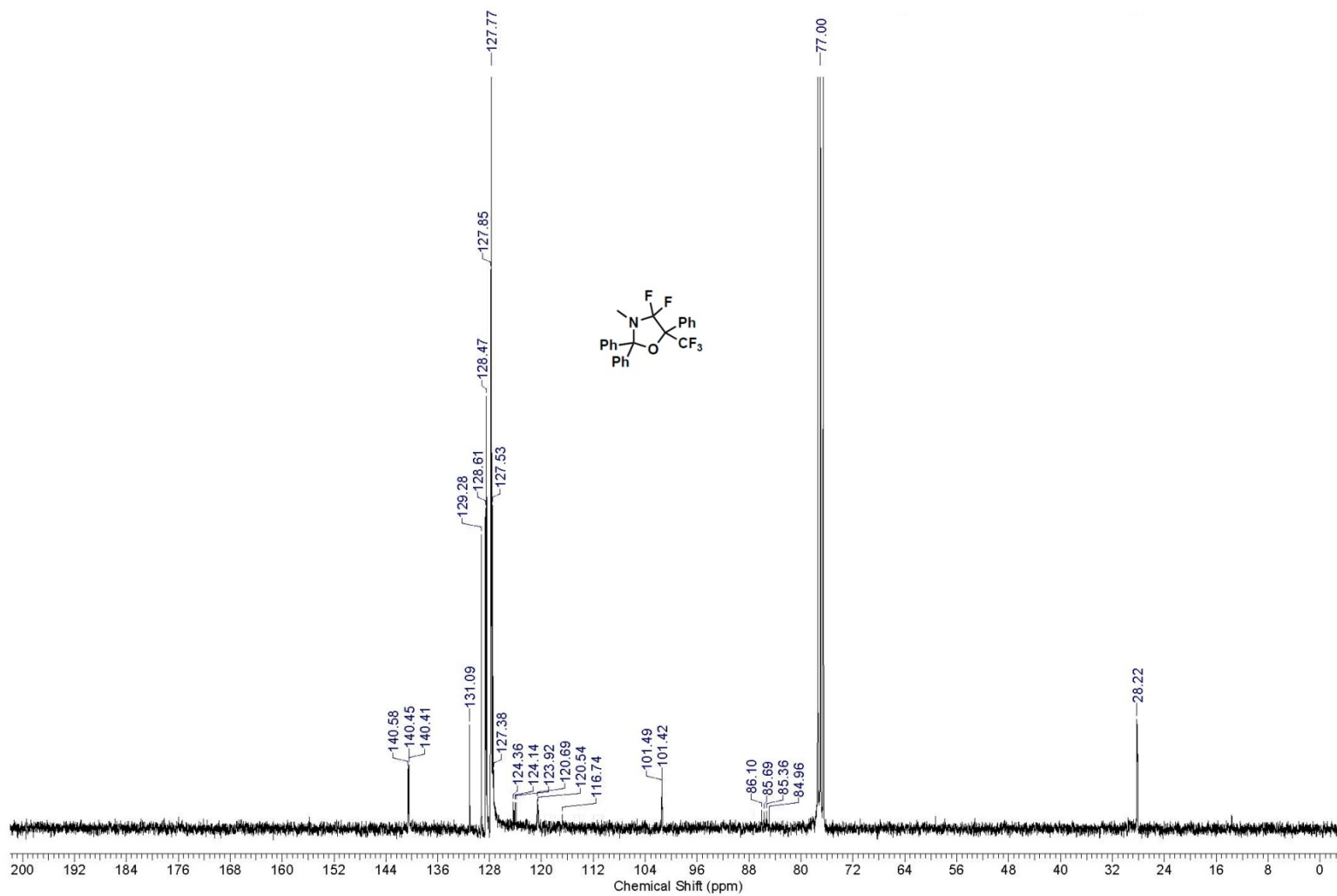
4-(3-Methyl-4-oxo-2,2-diphenyloxazolidin-5-yl)benzonitrile (14e), 75(¹³C) MHz, CDCl₃



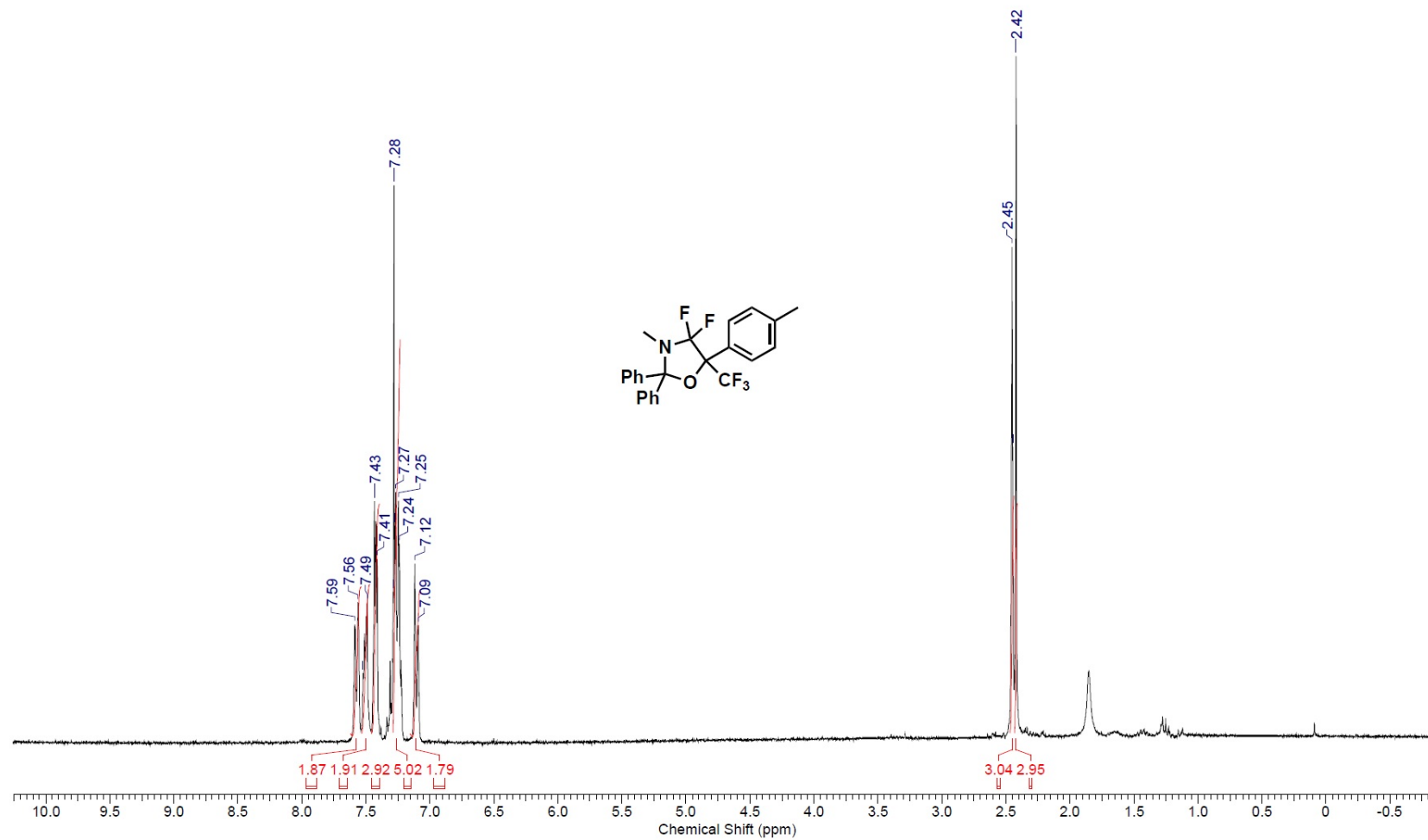
4,4-Difluoro-3-methyl-2,2,5-triphenyl-5-(trifluoromethyl)oxazolidine (28a), 300(¹H) MHz, CDCl₃



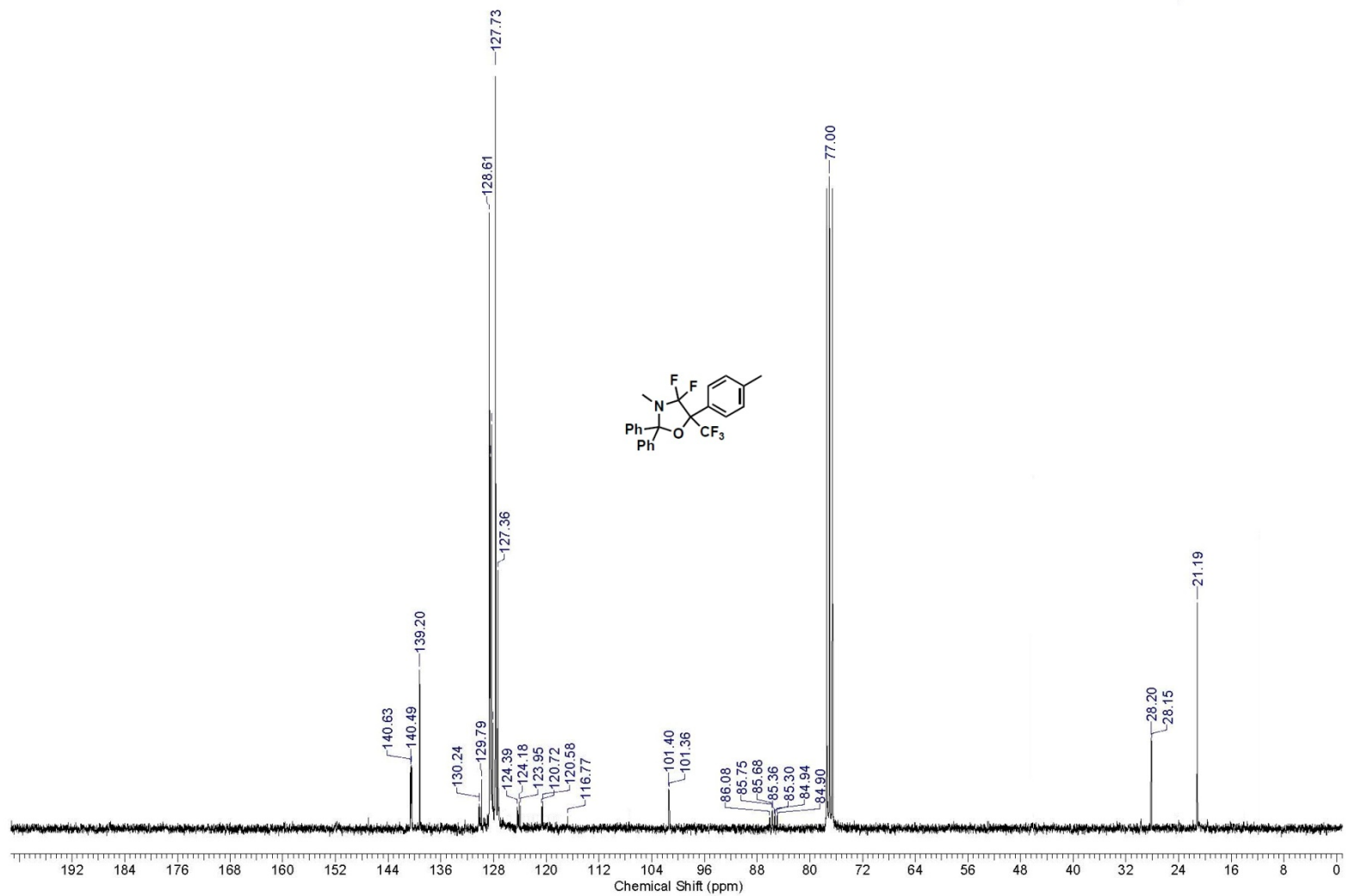
4,4-Difluoro-3-methyl-2,2,5-triphenyl-5-(trifluoromethyl)oxazolidine (28a), 75(¹³C) MHz, CDCl₃



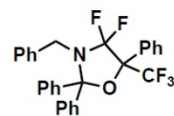
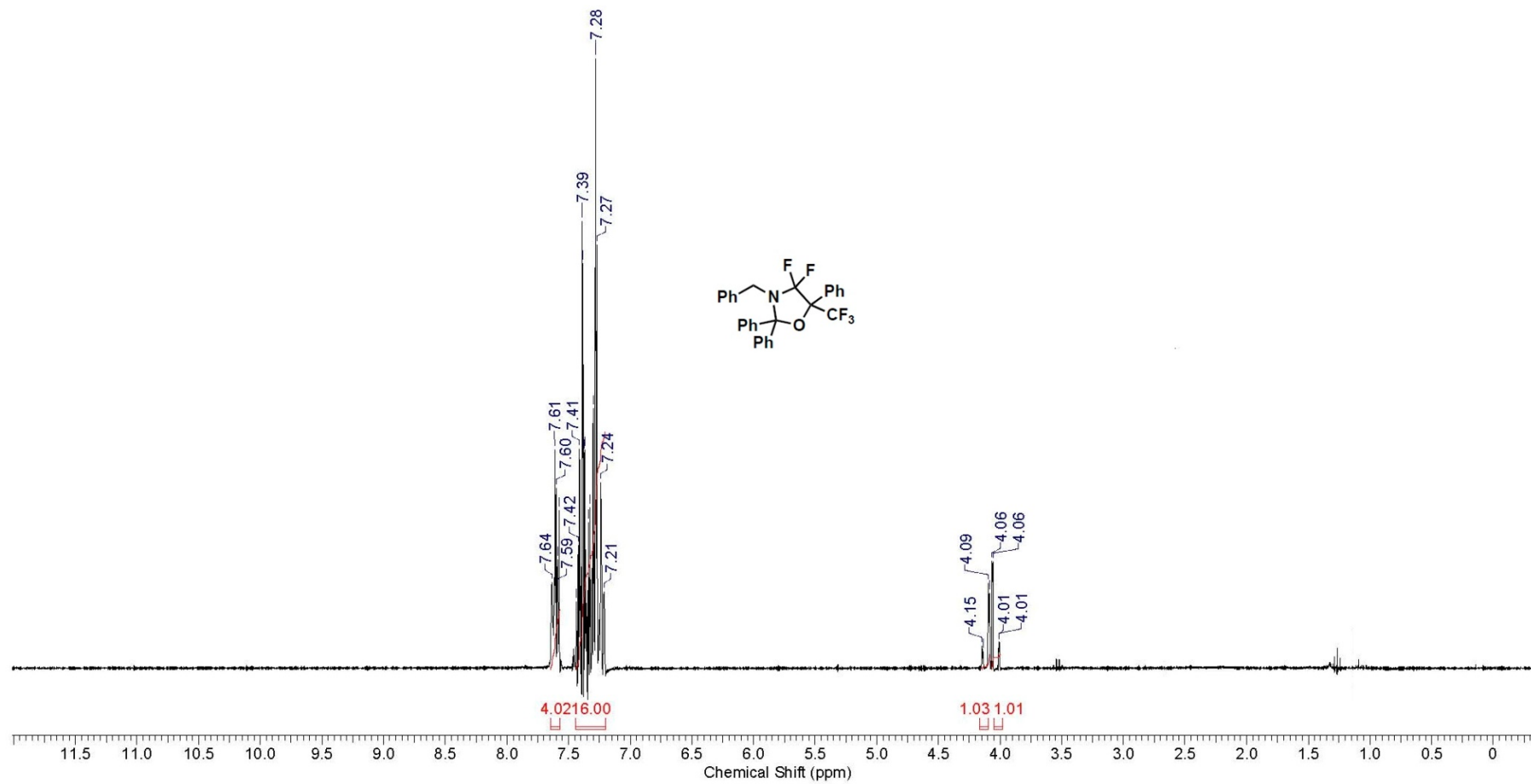
4,4-Difluoro-3-methyl-2,2-diphenyl-5-(p-tolyl)-5-(trifluoromethyl)oxazolidine (28b), 300(¹H) MHz, CDCl₃



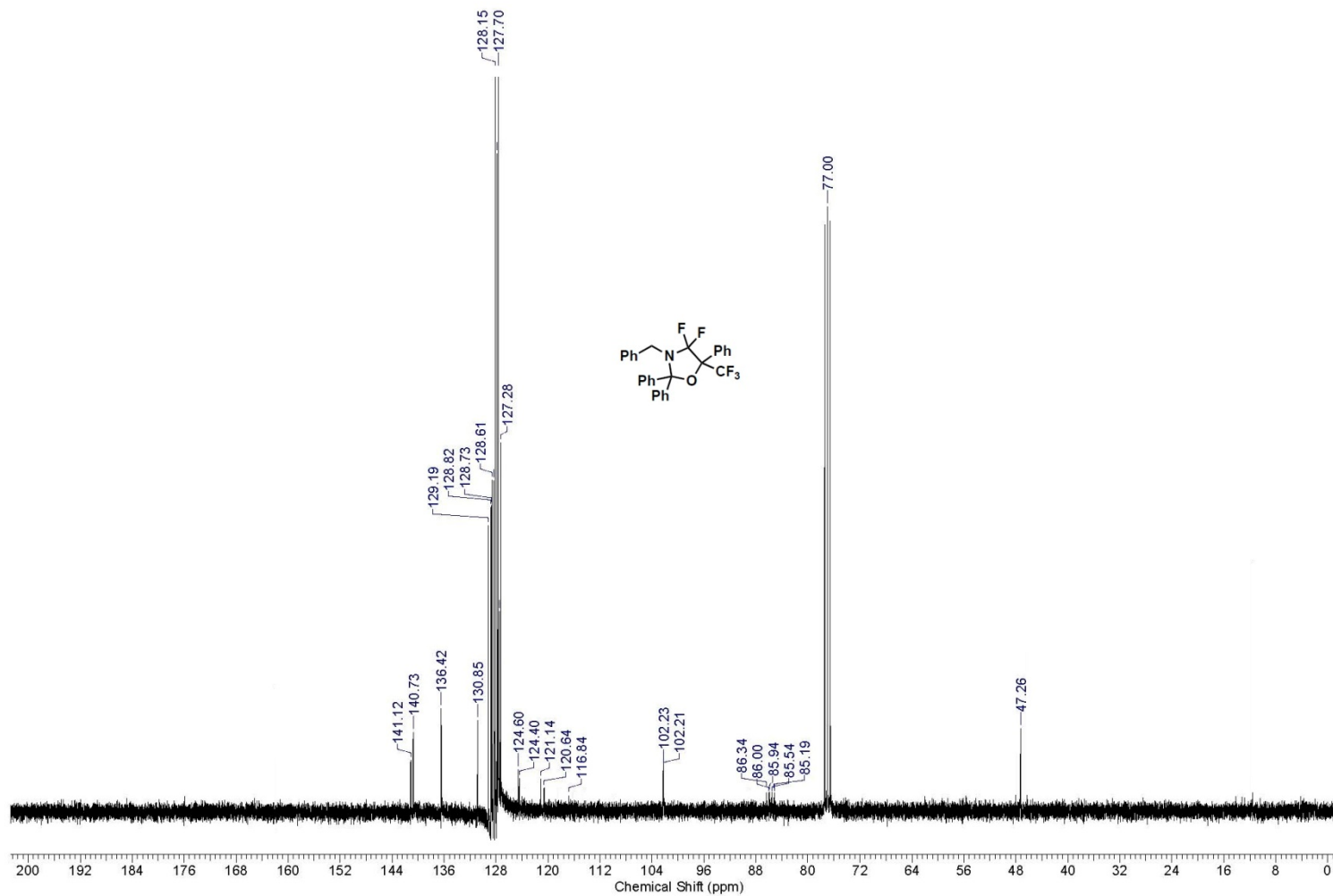
4,4-Difluoro-3-methyl-2,2-diphenyl-5-(p-tolyl)-5-(trifluoromethyl)oxazolidine (28b), 75(¹³C) MHz, CDCl₃



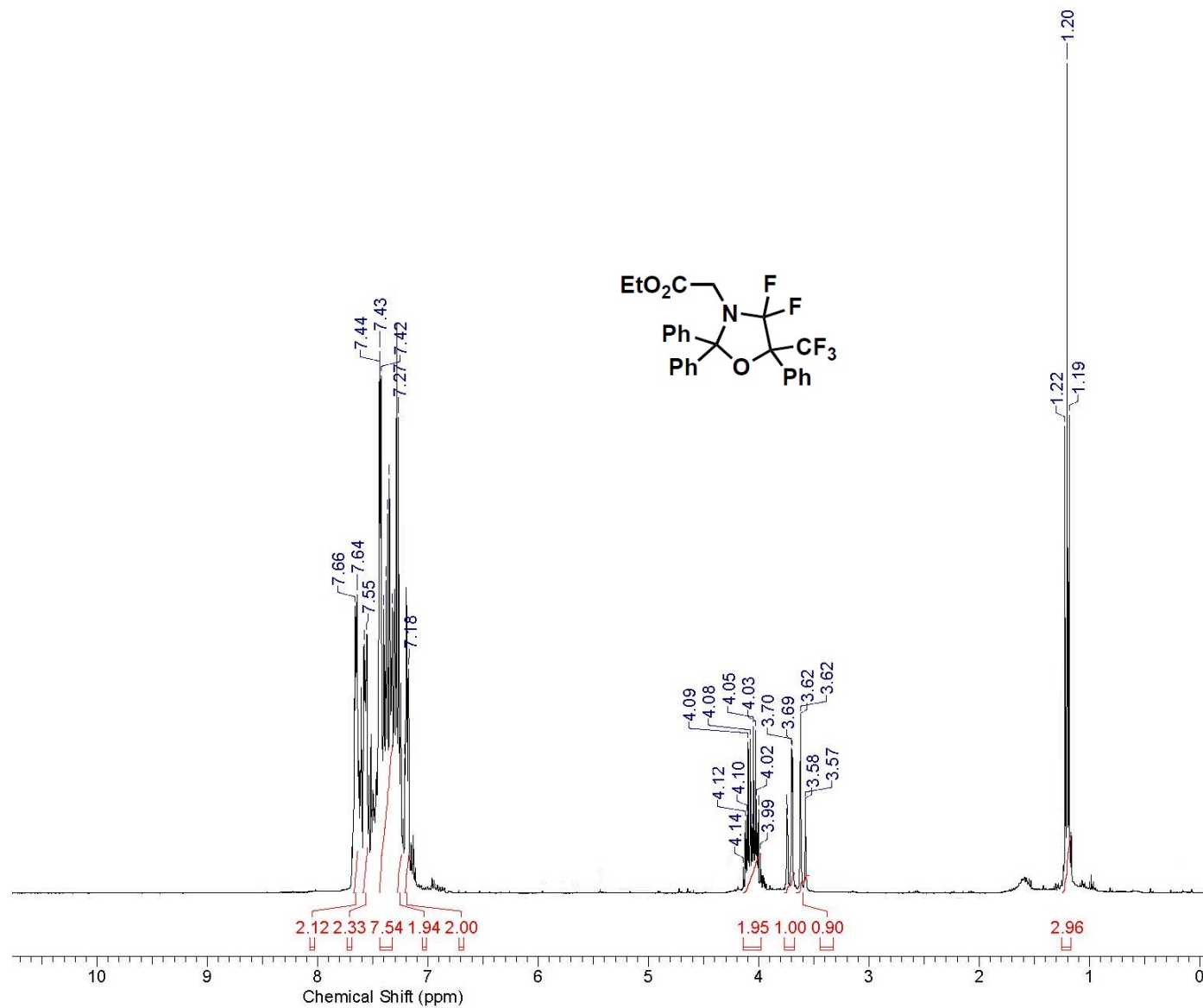
3-Benzyl-4,4-difluoro-2,2,5-triphenyl-5-(trifluoromethyl)oxazolidine (28c), 300(¹H) MHz, CDCl₃



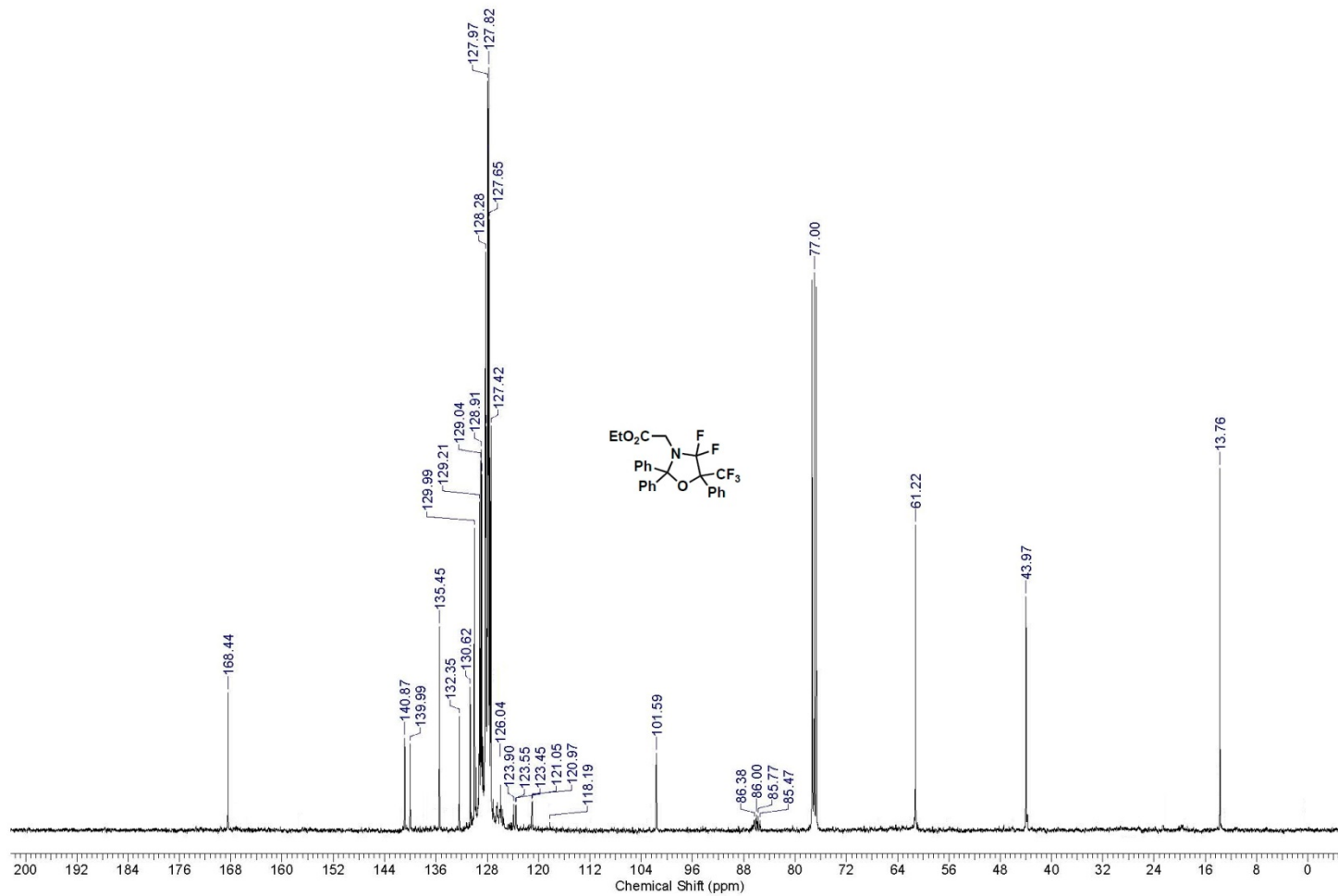
3-Benzyl-4,4-difluoro-2,2,5-triphenyl-5-(trifluoromethyl)oxazolidine (28c), 75(¹³C) MHz, CDCl₃



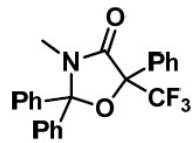
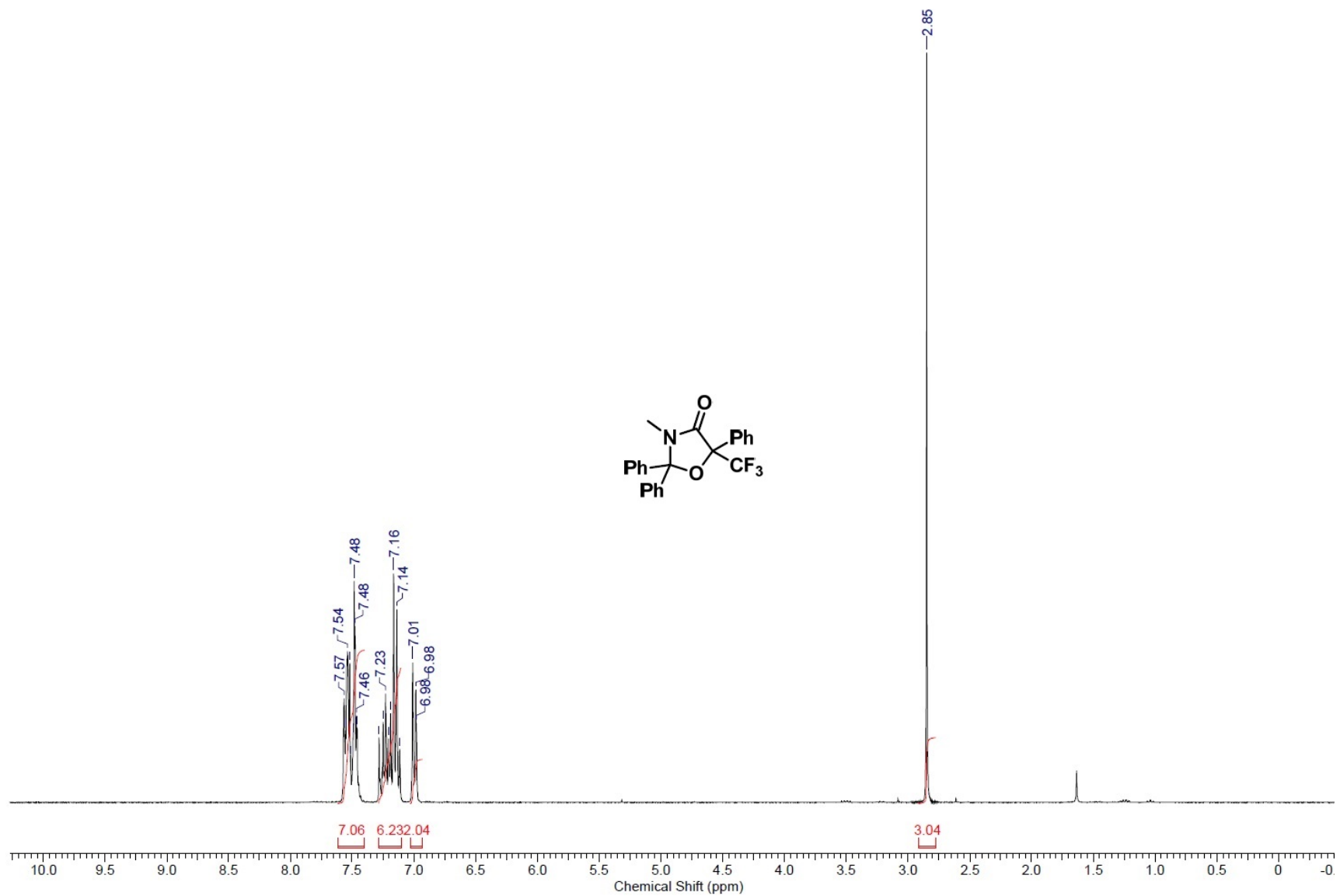
Ethyl 2-(4,4-difluoro-5-(trifluoromethyl)-2,2,5-triphenyloxazolidin-3-yl)acetate (28d), 400(¹H) MHz, CDCl₃



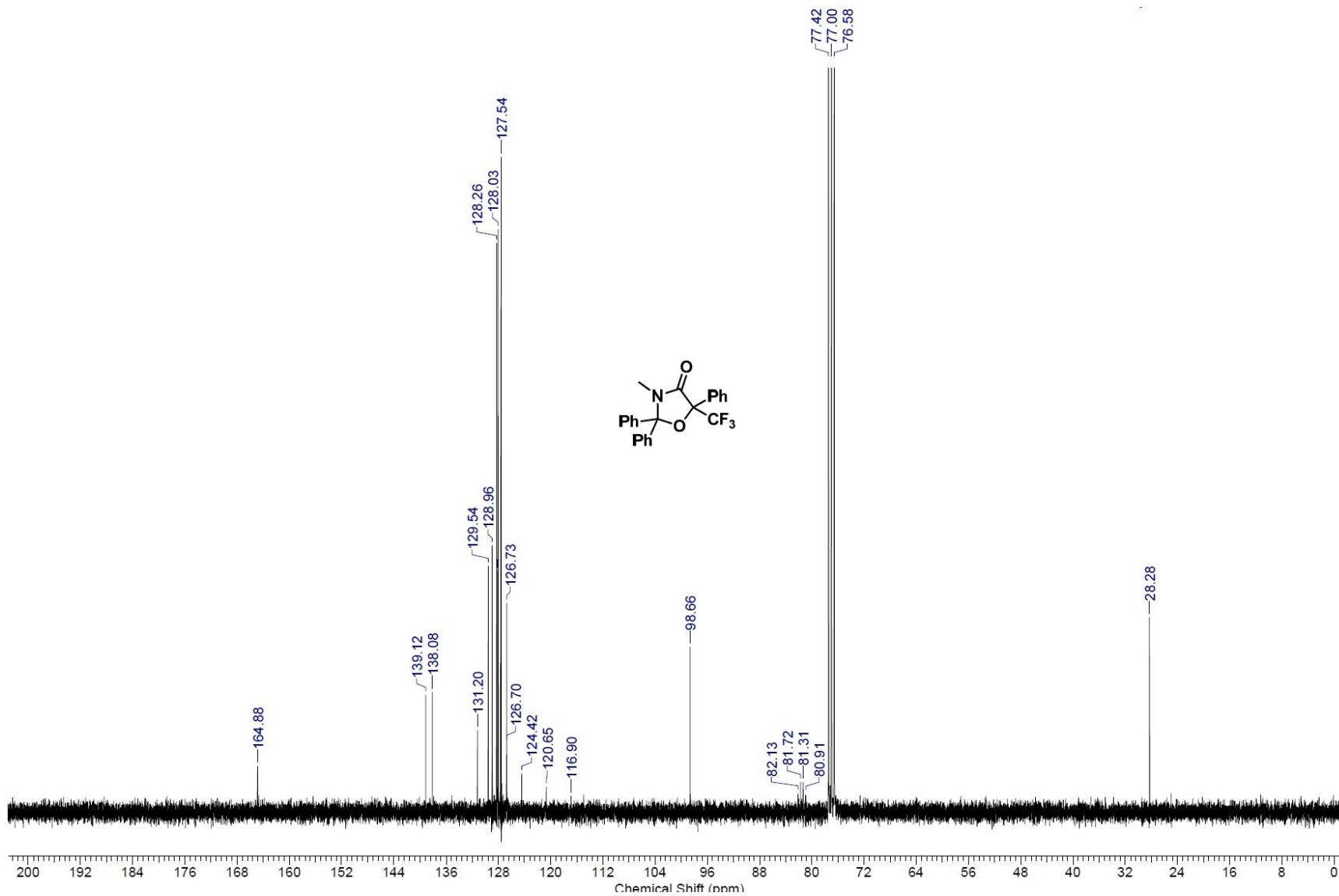
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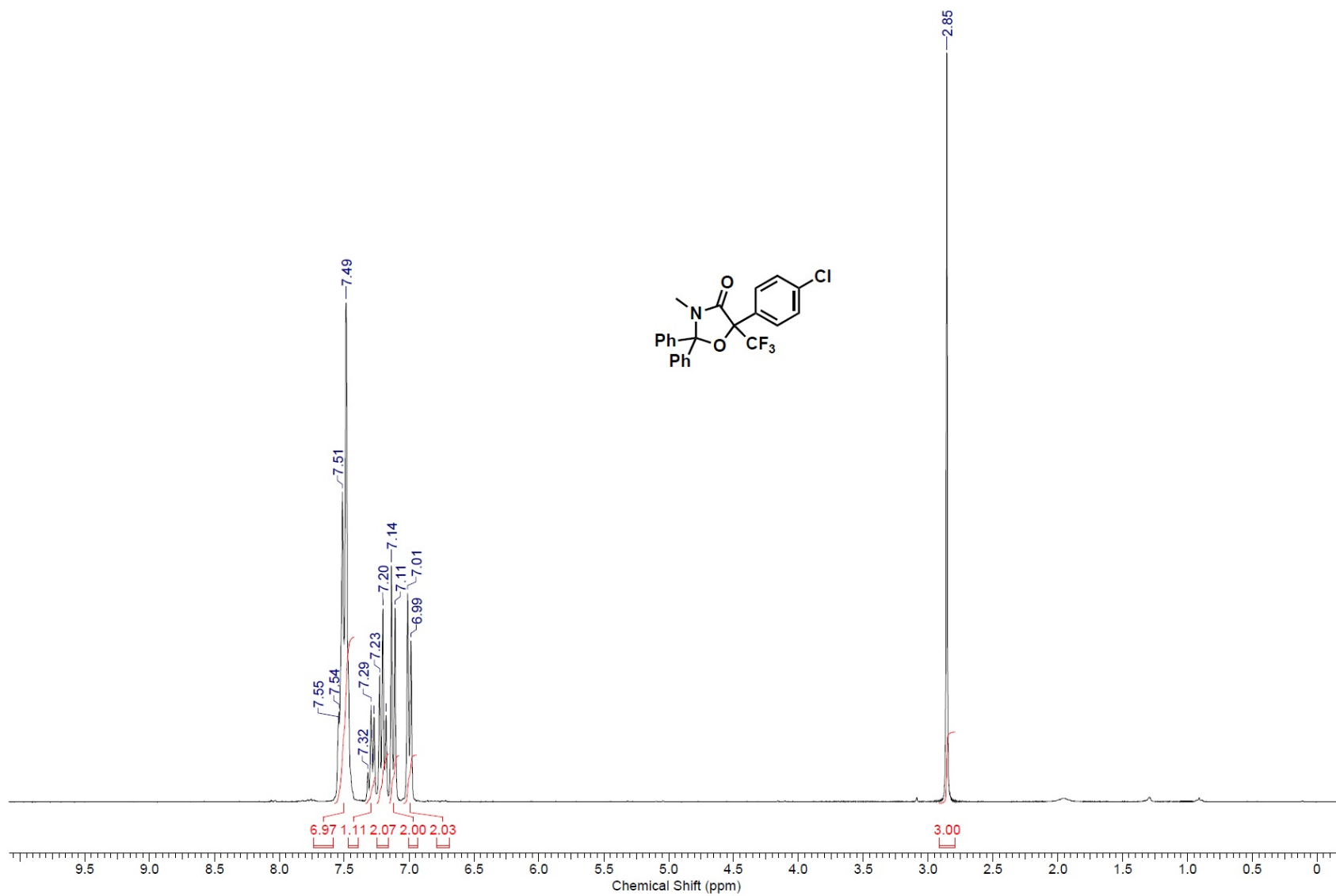
3-Methyl-2,2,5-triphenyl-5-(trifluoromethyl)oxazolidin-4-one (29a), 300(¹H) MHz, CDCl₃



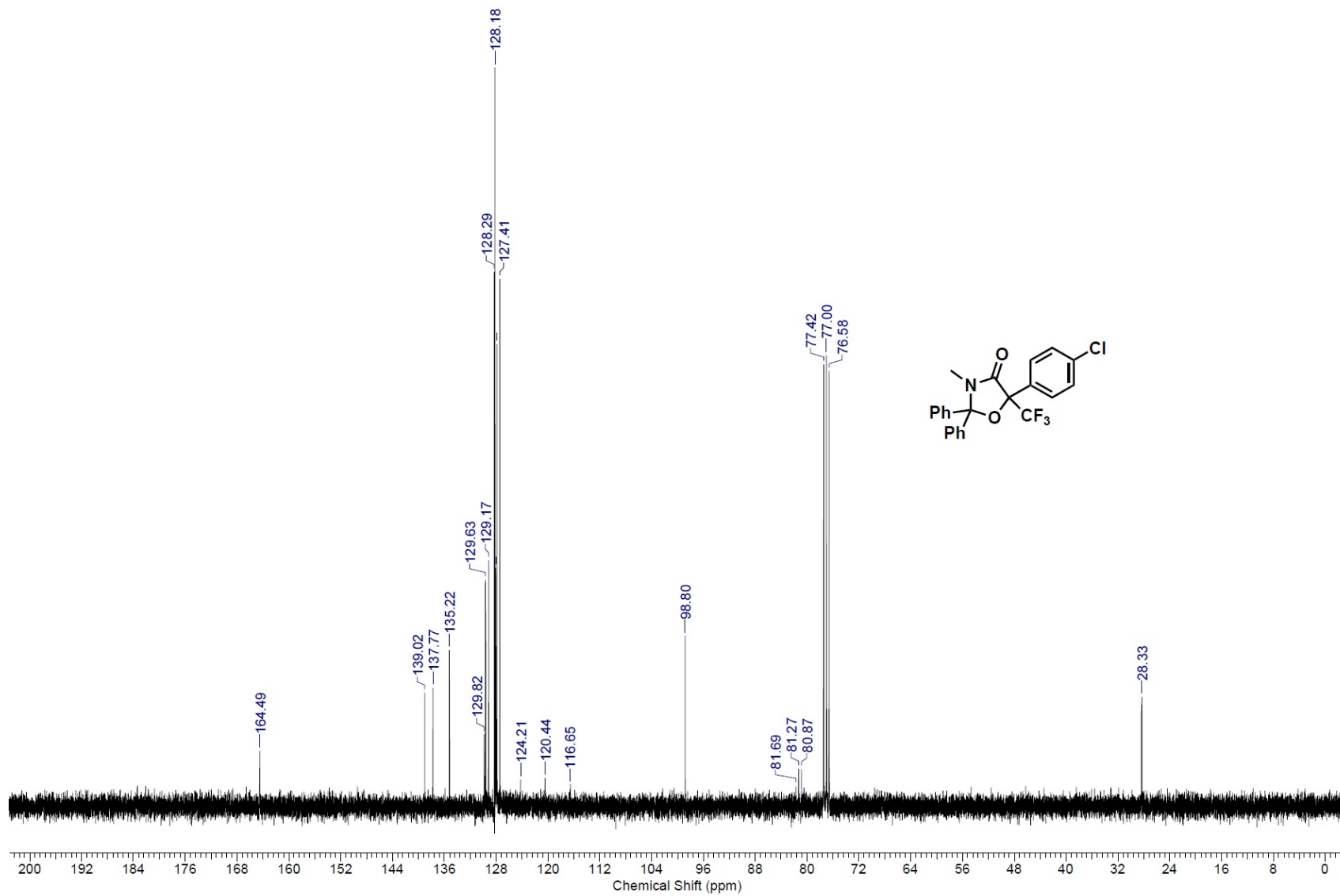
3-Methyl-2,2,5-triphenyl-5-(trifluoromethyl)oxazolidin-4-one (29a), 75(¹³C) MHz, CDCl₃



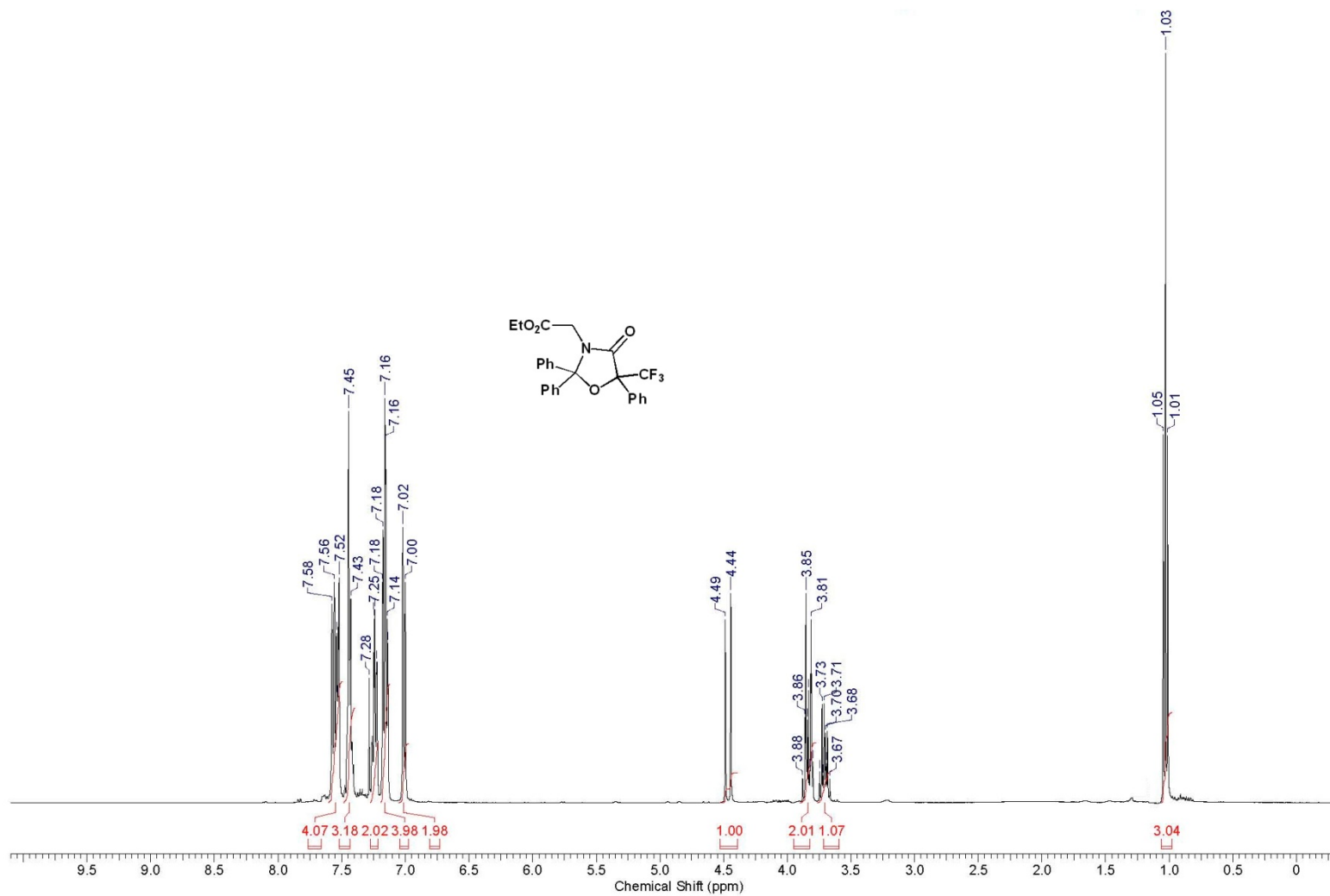
5-(4-Chlorophenyl)-3-methyl-2,2-diphenyl-5-(trifluoromethyl)oxazolidin-4-one (29b), 300(¹H) MHz, CDCl₃



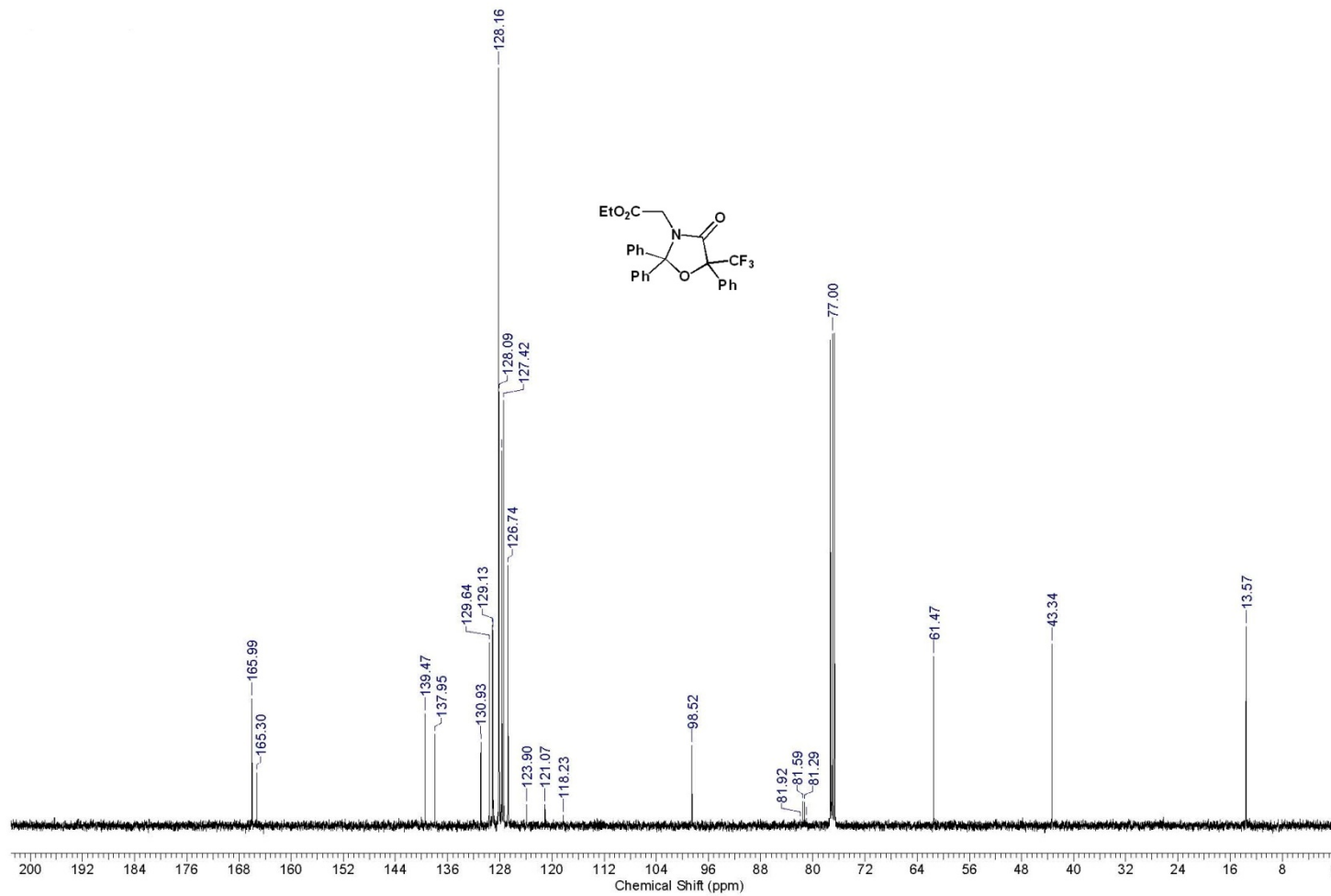
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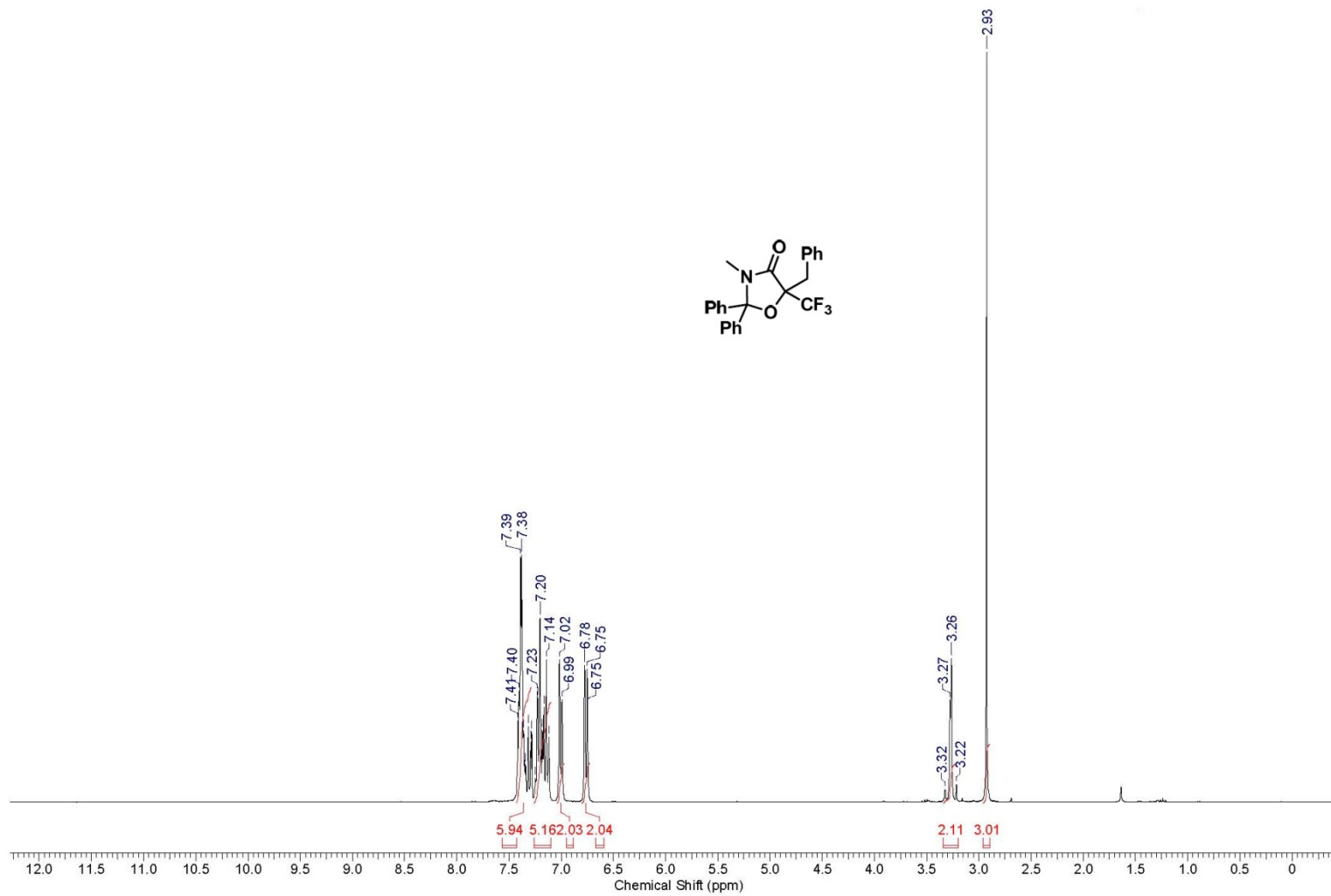
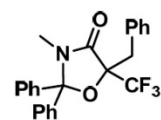
Ethyl 2-(4-oxo-2,2,5-triphenyl-5-(trifluoromethyl)oxazolidin-3-yl)acetate (29c), 400(¹H) MHz, CDCl₃



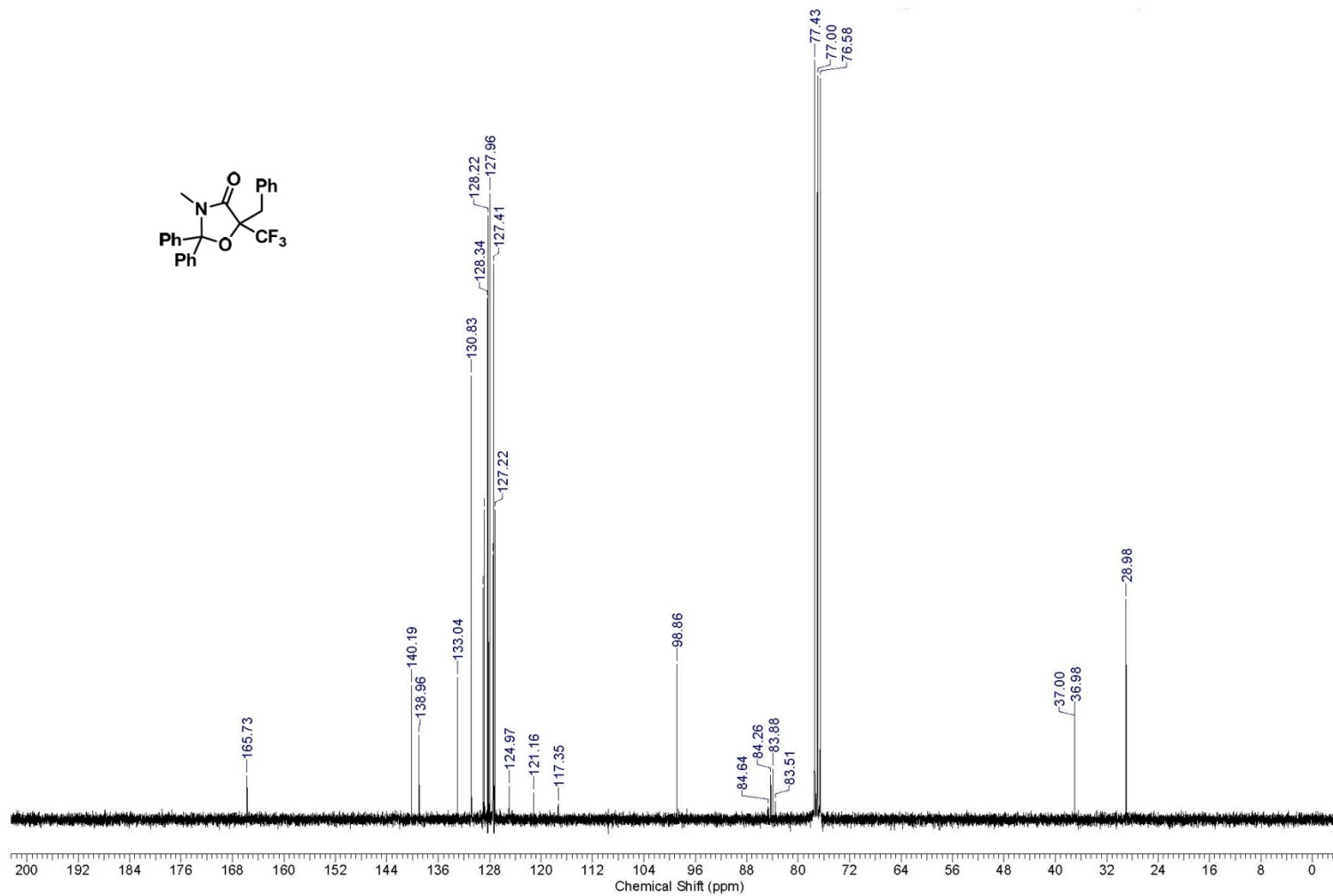
Ethyl 2-(4-oxo-2,2,5-triphenyl-5-(trifluoromethyl)oxazolidin-3-yl)acetate (29c), 100(¹H) MHz, CDCl₃



5-Benzyl-3-methyl-2,2-diphenyl-5-(trifluoromethyl)oxazolidin-4-one (29d), 300(¹H) MHz, CDCl₃



5-Benzyl-3-methyl-2,2-diphenyl-5-(trifluoromethyl)oxazolidin-4-one (29d), 75(¹³C) MHz, CDCl₃



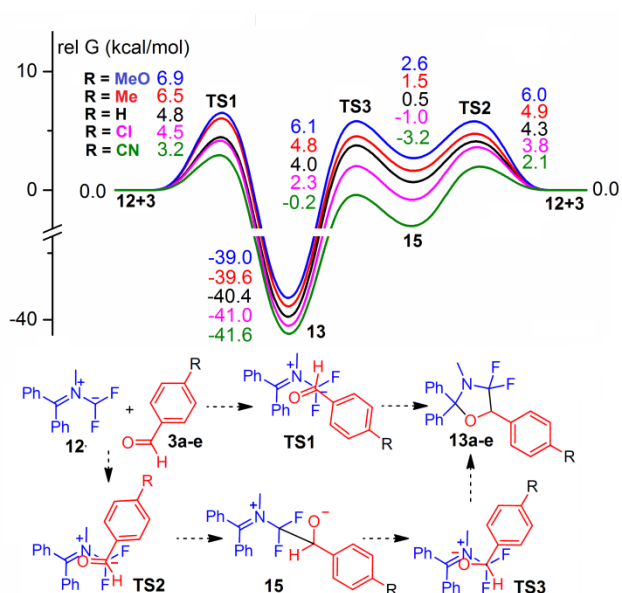


Figure 3 Energy profiles for the reaction of ylide **12** and benzaldehydes **3a–e**. Relative free *Gibbs* energies (in kcal mol⁻¹, 298 K, PCM model for DCM) computed at the DFT B3LYP/6-31G(d).

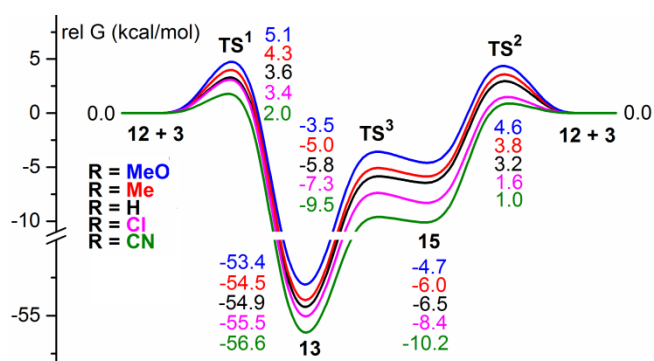


Figure S3-1 Energy profiles for the reaction of ylide **12** and benzaldehydes **3a–e**. Relative free *Gibbs* energies (in kcal mol⁻¹, 298 K, PCM model for DCM), single point calculation at the DFT wb97XD/6-311G(d,p) level with B3LYP/6-31G(d) optimized geometries.

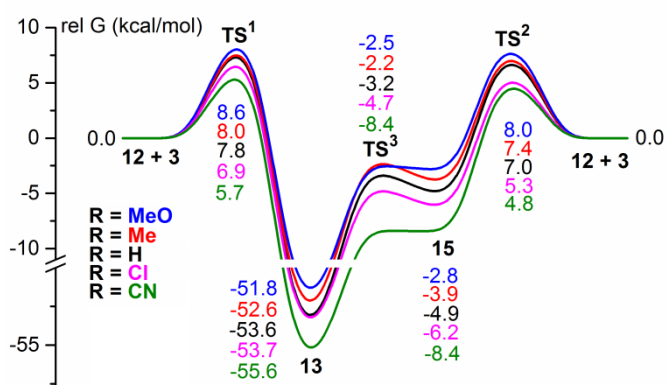


Figure S3-2 Energy profiles for the reaction of ylide **12** and benzaldehydes **3a–e**. Relative free *Gibbs* energies (in kcal mol⁻¹, 298 K, PCM model for DCM), single point calculation at the DFT MPWB1K/6-311G(d,p) level with B3LYP/6-31G(d) optimized geometries.

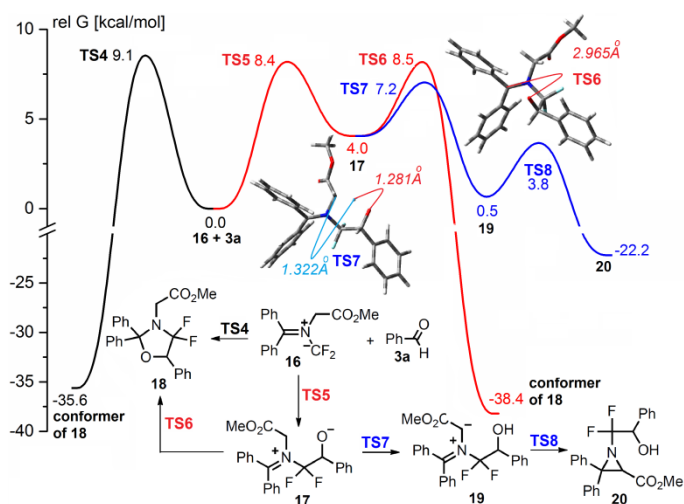


Figure 4 Energy profiles for the transformations of **16**. Relative free *Gibbs* energies (in kcal mol⁻¹, 298 K, PCM model for DCM) computed at the DFT B3LYP/6-31G(d) level.

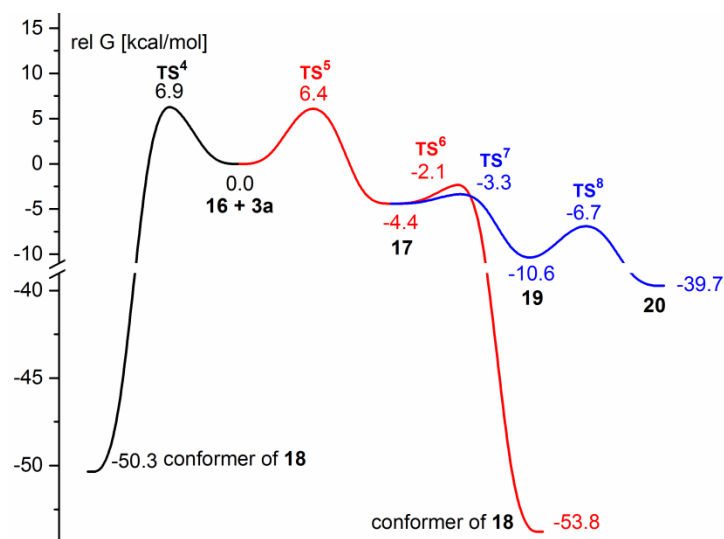


Figure S4-1 Energy profiles for the transformations of **16**. Relative free *Gibbs* energies (in kcal mol⁻¹, 298 K, PCM model for DCM), single point calculation at the DFT MPWB1K/6-311G(d,p) level with B3LYP/6-31G(d) optimized geometries.

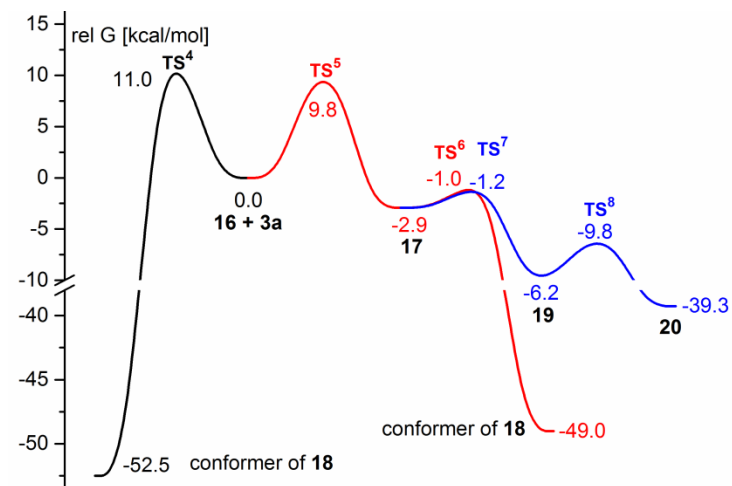


Figure S4-2 Energy profiles for the transformations of **16**. Relative free *Gibbs* energies (in kcal mol⁻¹, 298 K, PCM model for DCM), single point calculation at the DFT wB97XD/6-311G(d,p) level with B3LYP/6-31G(d) optimized geometries.

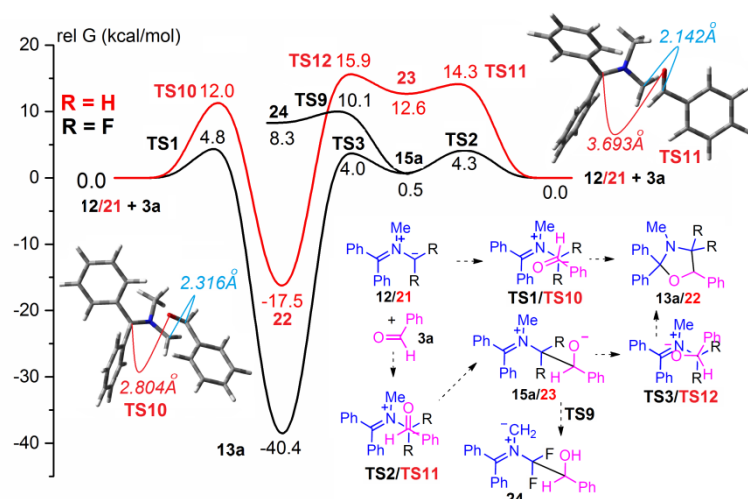


Figure 5 Energy profiles for the reactions of benzaldehyde **3a** with fluorinated ylide **12** and non-fluorinated ylide **21**. Relative free *Gibbs* energies (in kcal mol⁻¹, 298 K, PCM model for DCM) computed at the DFT B3LYP/6-31G(d) level.

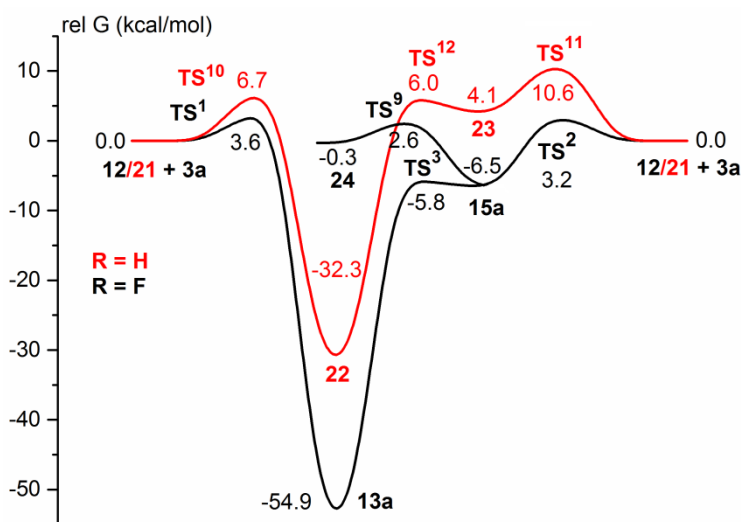


Figure S5-1 Energy profiles for the reactions of benzaldehyde **3a** with fluorinated ylide **12** and non-fluorinated ylide **21**. Relative free *Gibbs* energies (in kcal mol⁻¹, 298 K, PCM model for DCM), single point calculation at the DFT wB97XD/6-311G(d,p) level with B3LYP/6-31G(d) optimized geometries.

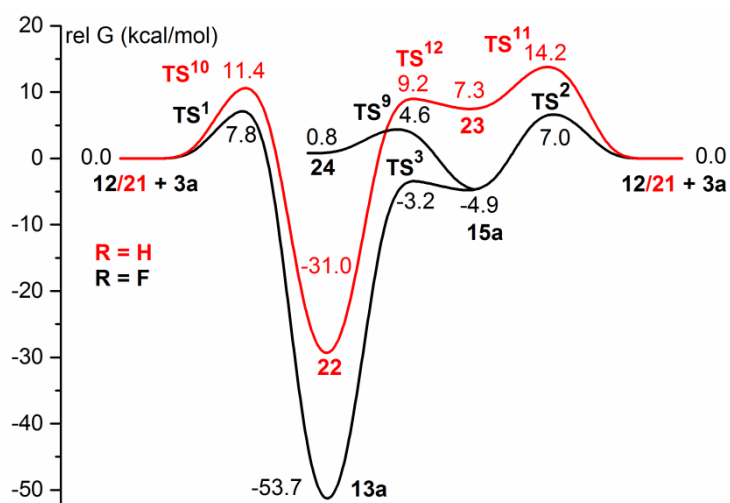


Figure S5-2 Energy profiles for the reactions of benzaldehyde **3a** with fluorinated ylide **12** and non-fluorinated ylide **21**. Relative free *Gibbs* energies (in kcal mol⁻¹, 298 K, PCM model for DCM), single point calculation at the DFT MPWB1K/6-311G(d,p) level with B3LYP/6-31G(d) optimized geometries.

Computational Details

All calculations were performed with the B3LYP density functional method¹ by using the Gaussian 09 suite of quantum chemical programs² at Resource center "Computer center of Saint Petersburg State University". Geometry optimizations of intermediates, transition states, reactants, and products in dichloromethane were performed at the DFT B3LYP/6-31G(d) level using PCM model.³ Stationary points on the respective potential-energy surfaces were characterized at the same level of theory by evaluating the corresponding Hessian indices. Careful verification of the unique imaginary frequencies for transition states was carried out to check whether the frequency indeed pertains to the desired reaction coordinate.

Table 2. B3LYP/6-31G(d) Absolute Energies (au), Cartesian Coordinates of stationary points

Molecule 3a				Molecule 3b			
E = -345.57857499, H (0K) = -345.468308, H (298K) = -345.461065, G (298K) = -345.498856 au. Imaginary frequency = 0.				E = -384.89766830, H (0K) = -384.759965, H (298K) = -384.750840, G (298K) = -384.793839 au Imaginary frequency = 0.			
O	-2.8516140	-0.3953040	-0.0000620	O	3.3173990	-0.5498270	0.0015970
C	-1.9888660	0.4684650	0.0000450	C	2.5128960	0.3699440	0.0011480
C	-0.5351790	0.2106920	0.0000220	C	1.0484360	0.2115830	0.0001980
C	0.3573470	1.2922130	-0.0000050	C	0.2250540	1.3450880	-0.0005100
C	1.7328960	1.0637050	-0.0000150	C	-1.1617320	1.2062470	-0.0020880
C	2.2176060	-0.2470100	-0.0000110	C	-1.7557900	-0.0633870	-0.0024420
C	1.3303500	-1.3312440	0.0000040	C	-0.9198840	-1.1969650	-0.0026360
C	-0.0420690	-1.1047440	0.0000270	C	0.4611960	-1.0658200	-0.0009430
H	-2.2690920	1.5433170	0.0001300	H	2.8650030	1.4235610	0.0015920
H	-0.0306280	2.3083130	-0.0000180	H	0.6733340	2.3362210	-0.0006880
H	2.4245910	1.9009090	-0.0000400	H	-1.7923430	2.0914510	-0.0033090
H	3.2891470	-0.4265420	-0.0000280	H	-1.3675880	-2.1879420	-0.0045830
H	1.7150660	-2.3469810	0.0000030	H	1.1065550	-1.9390470	-0.0013820
H	-0.7486770	-1.9290460	0.0000560	C	-3.2560810	-0.2238560	0.0031130
Molecule 3c				Molecule 3d			
E = -460.10567052, H (0K) = -459.962661, H (298K) = -459.952859, G (298K) = -459.996700 au. Imaginary frequency = 0.				E = -805.17408590, H (0K) = -805.073532, H (298K) = -805.065104, G (298K) = -805.106292 au. Imaginary frequency = 0.			
O	-3.7857230	-0.3285060	-0.0005420	O	3.6912570	-0.5981790	0.0000290
C	-2.8992490	0.5149870	-0.0000670	C	2.9127720	0.3413380	-0.0000180
C	-1.4601170	0.2293570	0.0001320	C	1.4413650	0.2117740	-0.0000130
C	-0.5377720	1.2839690	0.0002730	C	0.8371320	-1.0552530	-0.0000150
C	0.8339630	1.0426670	0.0003390	C	-0.5471090	-1.1743420	-0.0000070
C	1.2961320	-0.2830050	0.0002480	C	-1.3237970	-0.0104770	0.0000020
C	0.3757920	-1.3524160	0.0002120	C	-0.7474560	1.2604140	0.0000010

¹ (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648–5652. (b) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098–3100. (c) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785–789.

² Gaussian 09, Revision D.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, 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, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, **2013**.

³ J. Tomasi, B. Mennucci, and R. Cammi, *Chem. Rev.*, **2005**, *105*, 2999–3093.

C	-0.9819920	-1.0966390	0.0001380	C	0.6420420	1.3629370	-0.0000050
H	-3.1552410	1.5963270	0.0001350	H	3.2876260	1.3861720	0.0000160
H	-0.8982050	2.3103600	0.0004110	H	1.4675980	-1.9387300	-0.0000230
H	1.5268360	1.8752780	0.0005850	H	-1.0238230	-2.1483660	-0.0000100
H	0.7622430	-2.3668020	0.0001700	H	-1.3728380	2.1460760	0.0000060
H	-1.6988560	-1.9120850	-0.0000140	H	1.1081540	2.3450400	-0.0000020
O	2.6022380	-0.6399770	0.0003430	Cl	-3.0756740	-0.1543000	0.0000070
C	3.5963090	0.3863110	-0.0007200				
H	3.5197070	1.0129900	0.8950560				
H	4.5552760	-0.1326130	-0.0017910				
H	3.5177180	1.0130330	-0.8962830				
Molecule 3e				Molecule 12			
E = -437.82265207, H (0K) = -437.713889,				E = -833.76699090, H (0K) = -833.523656,			
H (298K) = -437.704852, G (298K) = -437.747183 au				H (298K) = -833.507267, G (298K) = -833.567102 au			
Imaginary frequency = 0.				Imaginary frequency = 0.			
O	3.5658890	-0.6076260	0.0000270	C	-0.0260250	0.3501370	0.0466900
C	2.7957800	0.3364080	-0.0000150	C	1.5606280	2.2140670	0.1843330
C	1.3184360	0.2078190	-0.0000130	N	0.2616460	1.6499850	0.2175630
C	0.7186370	-1.0611080	-0.0000150	C	-0.7644380	2.6022220	0.7211930
C	-0.6638230	-1.1784190	-0.0000060	F	2.2755380	1.6461500	-0.8484620
C	-1.4577190	-0.0147220	0.0000020	F	1.4425200	3.5570750	-0.1473130
C	-0.8635750	1.2586750	0.0000000	C	1.0008370	-0.7065710	-0.0408210
C	0.5239610	1.3621490	-0.0000060	C	0.7367590	-1.8706080	-0.7910130
H	3.1739050	1.3790910	0.0000280	C	1.6361410	-2.9351970	-0.8025050
H	1.3518650	-1.9421170	-0.0000250	C	2.8058580	-2.8763840	-0.0424570
H	-1.1374440	-2.1542240	-0.0000090	C	3.0724030	-1.7343180	0.7205530
H	-1.4860600	2.1466840	0.0000030	C	2.1961390	-0.6545220	0.7070080
H	0.9935120	2.3421060	-0.0000010	C	-1.4486110	-0.0821980	0.0477800
C	-2.8874540	-0.1311530	0.0000060	C	-1.8864340	-1.0953590	0.9207780
N	-4.0469070	-0.2269190	0.0000100	C	-3.2130330	-1.5219290	0.9051210
				C	-4.1222820	-0.9584180	0.0052500
				C	-3.6970970	0.0358860	-0.8786180
				C	-2.3722780	0.4711530	-0.8579660
				H	-0.2943430	3.2377550	1.4696290
				H	-1.5897310	2.0560170	1.1673290
				H	-1.1214170	3.2256810	-0.1000350
				H	-0.1765950	-1.9352200	-1.3734180
				H	1.4184230	-3.8133260	-1.4042600
				H	3.5066080	-3.7066030	-0.0487900
				H	3.9772110	-1.6796440	1.3200090
				H	2.4263340	0.2369420	1.2815660
				H	-1.1826880	-1.5378940	1.6190870
				H	-3.5375620	-2.2949110	1.5960310
				H	-5.1545050	-1.2966840	-0.0103000
				H	-4.3942770	0.4689080	-1.5903170
				H	-2.0429130	1.2322980	-1.5594480
TS¹ 3a+12				TS¹ 3b+12			
E = -1179.35834055, H (0K) = -1179.003458,				E = -1218.67730386, H (0K) = -1218.294293,			
H (298K) = -1178.979905, G (298K) = -1179.058322 au				H (298K) = -1218.269292, G (298K) = -1218.350645 au			
Imaginary frequency = 1.				Imaginary frequency = 1.			
C	1.4505190	0.0798930	0.4667350	C	1.6827090	0.1469950	0.4505920
O	-1.1055360	-2.0879110	-1.0394350	O	-0.8123390	-2.7251490	0.2098610
C	-1.9499740	-1.8553490	-0.1680100	C	-1.6074340	-1.9850450	0.8289420
C	-0.9203220	-0.0182350	1.1486430	C	-0.5184900	-0.1340040	1.5293250
N	0.4549330	-0.3811080	1.2452440	N	0.8829800	-0.3920580	1.3846990
C	0.6379820	-1.5817870	2.0896460	C	1.2912390	-1.5833910	2.1641760
F	-1.4585390	0.2334150	2.3860960	F	-0.8466390	0.0639430	2.8473610
F	-1.1317180	1.0835450	0.3954460	F	-0.9248130	0.9651700	0.8573520
C	-3.1840390	-1.0609150	-0.4092640	C	-2.7157910	-1.2544530	0.1405840

C	-4.1855790	-1.0034440	0.5702350	C	-3.7280670	-0.6288070	0.8802430
C	-5.3584400	-0.2866120	0.3364840	C	-4.7771170	0.0236050	0.2365440
C	-5.5368550	0.3796500	-0.8798480	C	-4.8477120	0.0692720	-1.1643390
C	-4.5402690	0.3254710	-1.8610510	C	-3.8285880	-0.5583610	-1.8980630
C	-3.3695880	-0.3921830	-1.6278110	C	-2.7795260	-1.2135320	-1.2579960
C	1.5116010	1.4969230	0.0930300	C	1.5802730	1.5695900	0.1076180
C	2.0747860	1.8886420	-1.1396180	C	1.8594720	2.0148950	-1.2010520
C	2.1806090	3.2344280	-1.4776660	C	1.8109640	3.3699970	-1.5142370
C	1.7362670	4.2201420	-0.5905790	C	1.4955940	4.3090300	-0.5272190
C	1.1827240	3.8490870	0.6376760	C	1.2248440	3.8838830	0.7764520
C	1.0679710	2.5039770	0.9771320	C	1.2623470	2.5292750	1.0924210
C	2.5229090	-0.8391840	0.0289000	C	2.6965580	-0.6939520	-0.2143970
C	3.8739550	-0.4628560	0.1611500	C	4.0160640	-0.2282240	-0.3762060
C	4.8930630	-1.3238740	-0.2405890	C	4.9719830	-1.0188120	-1.0096190
C	4.5829900	-2.5702450	-0.7918080	C	4.6245460	-2.2794650	-1.5037560
C	3.2456810	-2.9474830	-0.9424630	C	3.3145190	-2.7455070	-1.3610090
C	2.2207490	-2.0935060	-0.5385520	C	2.3533110	-1.9641780	-0.7226940
H	-1.9541220	-2.4184210	0.7852780	H	-1.7948800	-2.1514060	1.9087300
H	0.0178320	-1.4519050	2.9766940	H	0.9414520	-1.4316010	3.1863930
H	1.6847080	-1.6511510	2.3801020	H	2.3765590	-1.6556900	2.1565240
H	0.3360810	-2.4881190	1.5634550	H	0.8355990	-2.4803400	1.7418060
H	-4.0384190	-1.5203250	1.5161920	H	-3.6844130	-0.6467910	1.9675690
H	-6.1323190	-0.2466660	1.0982200	H	-5.5535820	0.5060130	0.8263170
H	-6.4504320	0.9386610	-1.0638300	H	-3.8629770	-0.5329650	-2.9853110
H	-4.6809790	0.8428850	-2.8063640	H	-1.9987720	-1.7073870	-1.8289230
H	-2.5870850	-0.4509820	-2.3781490	H	2.0948560	1.2898580	-1.9731550
H	2.4122590	1.1284760	-1.8365540	H	2.0157170	3.6948280	-2.5302690
H	2.6063750	3.5158790	-2.4366270	H	1.4658690	5.3670230	-0.7719130
H	1.8256890	5.2704990	-0.8532110	H	0.9895000	4.6098940	1.5493020
H	0.8450640	4.6097510	1.3358890	H	1.0730360	2.2049390	2.1107700
H	0.6598060	2.2234750	1.9429040	H	4.2905720	0.7469720	0.0139200
H	4.1195990	0.5014620	0.5955160	H	5.9888790	-0.6519390	-1.1161360
H	5.9299840	-1.0225120	-0.1208340	H	5.3694930	-2.8923280	-2.0035020
H	5.3781470	-3.2394310	-1.1085180	H	3.0364810	-3.7176340	-1.7585230
H	2.9982530	-3.9068080	-1.3889030	H	1.3281550	-2.3133650	-0.6326800
H	1.1812090	-2.3716070	-0.6905970	C	-6.0017000	0.7500670	-1.8621810
				H	-5.7022400	1.1448570	-2.8387510
				H	-6.8297090	0.0494070	-2.0358160
				H	-6.3986670	1.5779730	-1.2653190
TS¹ 3c+12				TS¹ 3d+12			
E = -1293.88391515, H (0K) = -1293.495681,				E = -1638.95593182, H (0K) = -1638.610273,			
H (298K) = -1293.469961, G (298K) = -1293.552749				H (298K) = -1638.585814, G (298K) = -1638.666238			
au				au			
Imaginary frequency = 1.				Imaginary frequency = 1.			
C	1.9642660	0.1793180	0.4373630	C	1.9152030	0.1783200	0.4239220
O	-0.3797280	-2.7660580	0.1423950	O	-0.4818930	-2.9121650	0.4706320
C	-1.1900660	-2.0921430	0.8217950	C	-1.2715930	-2.1747290	1.0862780
C	-0.2001800	-0.2485190	1.5411570	C	-0.1231330	-0.2164320	1.7577070
N	1.2117840	-0.4251610	1.3704930	N	1.2536340	-0.4191600	1.4291820
C	1.6941640	-1.6158980	2.1072270	C	1.8032960	-1.6049900	2.1267350
F	-0.5168060	-0.0990320	2.8682420	F	-0.2909660	-0.0728800	3.1126090
F	-0.6741500	0.8431550	0.9022580	F	-0.6521600	0.8858680	1.1806580
C	-2.3699140	-1.4167580	0.2009670	C	-2.3704520	-1.4308260	0.4024550
C	-3.4030620	-0.9035290	0.9912260	C	-3.3624550	-0.7802960	1.1482160
C	-4.5231780	-0.2966560	0.4212320	C	-4.4128860	-0.1182050	0.5167810
C	-4.6150320	-0.1969060	-0.9743560	C	-4.4604140	-0.1129810	-0.8780020
C	-3.5831020	-0.7112350	-1.7794390	C	-3.4874060	-0.7554320	-1.6455470
C	-2.4784880	-1.3128430	-1.1950710	C	-2.4465550	-1.4148250	-0.9964280
C	1.7811740	1.6024230	0.1320310	C	1.7228100	1.6058070	0.1468450
C	2.0172350	2.0928870	-1.1688460	C	1.8248570	2.1039140	-1.1687040
C	1.8937800	3.4507450	-1.4476090	C	1.6927030	3.4655350	-1.4241460

C	1.5453660	4.3478530	-0.4331560	C	1.4668040	4.3596910	-0.3729370
C	1.3165020	3.8778820	0.8632000	C	1.3701390	3.8824790	0.9371170
C	1.4286630	2.5198720	1.1448950	C	1.4928710	2.5208020	1.1966290
C	3.0122930	-0.5875970	-0.2632380	C	2.8567580	-0.6087930	-0.3947140
C	4.3031310	-0.0484230	-0.4280360	C	4.1255360	-0.0921060	-0.7234060
C	5.2901080	-0.7700390	-1.0952600	C	5.0110490	-0.8325350	-1.5028860
C	5.0017560	-2.0327540	-1.6211080	C	4.6423940	-2.0944940	-1.9780560
C	3.7198500	-2.5707530	-1.4756850	C	3.3814480	-2.6118900	-1.6688730
C	2.7282800	-1.8592550	-0.8031530	C	2.4916920	-1.8802110	-0.8847050
H	-1.3382070	-2.3245300	1.8963710	H	-1.4153380	-2.2903220	2.1770720
H	1.3495880	-1.5155230	3.1374970	H	1.5965510	-1.4731610	3.1900330
H	2.7816490	-1.6288170	2.0852740	H	2.8783620	-1.6416960	1.9658910
H	1.2815930	-2.5218790	1.6600880	H	1.3221880	-2.5144090	1.7641020
H	-3.3316750	-0.9738390	2.0748450	H	-3.3101130	-0.7880340	2.2345050
H	-5.3081020	0.0881460	1.0619550	H	-5.1818170	0.3846010	1.0934720
H	-3.6772010	-0.6287180	-2.8583550	H	-3.5488530	-0.7419870	-2.7286420
H	-1.6824780	-1.7230040	-1.8092930	H	-1.6831470	-1.9336700	-1.5675070
H	2.2785500	1.3997090	-1.9615270	H	1.9899340	1.4137740	-1.9894810
H	2.0659800	3.8102410	-2.4579700	H	1.7617970	3.8303990	-2.4448770
H	1.4573820	5.4084790	-0.6509310	H	1.3712410	5.4230640	-0.5734420
H	1.0558770	4.5718980	1.6570330	H	1.2045790	4.5734720	1.7586690
H	1.2717950	2.1613250	2.1572370	H	1.4399000	2.1571450	2.2179060
H	4.5317830	0.9289360	-0.0144210	H	4.4184870	0.8839070	-0.3490390
H	6.2849200	-0.3475170	-1.2040050	H	5.9904940	-0.4256190	-1.7377730
H	5.7705660	-2.5913000	-2.1476650	H	5.3317890	-2.6682260	-2.5910810
H	3.4873220	-3.5445090	-1.8976820	H	3.0843520	-3.5852940	-2.0491330
H	1.7234180	-2.2624080	-0.7090490	H	1.5024940	-2.2731670	-0.6658540
O	-5.6584190	0.3728830	-1.6426660	Cl	-5.7859430	0.7209970	-1.6905430
C	-6.7337410	0.9150940	-0.8815660				
H	-7.4423550	1.3142070	-1.6088310				
H	-7.2269890	0.1428360	-0.2787280				
H	-6.3909520	1.7240980	-0.2250460				
TS¹ 3e+12				Molecule 13a			
E = -1271.60685357, H (0K) = -1271.253066,				E = -1179.43731943, H (0K) = -1179.077362,			
H (298K) = -1271.227938, G (298K) = -1271.309189				H (298K) = -1179.055040, G (298K) = -1179.130281			
au				au			
Imaginary frequency = 1.				Imaginary frequency = 0.			
C	1.8049930	0.1824970	0.4294550	C	0.8422810	0.0822200	0.0696020
O	-0.6512340	-2.9772630	0.4615090	O	-0.3290400	-0.0112390	-0.7584420
C	-1.4490720	-2.2379430	1.0521200	C	-1.2938910	-0.8759800	-0.1506640
C	-0.2584710	-0.1761840	1.7339610	C	-0.9102020	-0.8629980	1.3465430
N	1.1171540	-0.4047540	1.4238380	N	0.2830710	-0.1506800	1.4157610
C	1.6413880	-1.5914890	2.1391230	C	1.0915200	-0.2476420	2.6217290
F	-0.4406830	-0.0003950	3.0830930	F	-0.8104590	-2.1664850	1.8210170
F	-0.7706980	0.9167510	1.1244420	F	-1.8748540	-0.3097760	2.1656660
C	-2.5033890	-1.4567430	0.3425810	C	-2.6959140	-0.4175280	-0.4681420
C	-3.4917140	-0.7771510	1.0695910	C	-3.6881330	-1.3628000	-0.7474450
C	-4.5010740	-0.0839560	0.4140590	C	-4.9972040	-0.9561350	-1.0158190
C	-4.5282250	-0.0660150	-0.9929660	C	-5.3194840	0.4019640	-1.0158480
C	-3.5414540	-0.7484920	-1.7291720	C	-4.3288760	1.3508660	-0.7447400
C	-2.5409260	-1.4403820	-1.0594530	C	-3.0241060	0.9439690	-0.4691280
C	1.6370410	1.6124950	0.1508100	C	1.3604360	1.5183540	-0.0788220
C	1.7711560	2.1112530	-1.1616570	C	2.3133800	1.8450180	-1.0511290
C	1.6603940	3.4746350	-1.4178620	C	2.7085780	3.1711500	-1.2396800
C	1.4230620	4.3701460	-0.3703610	C	2.1585620	4.1861610	-0.4550250
C	1.2936470	3.8923700	0.9366170	C	1.2027780	3.8687420	0.5132110
C	1.3958550	2.5291310	1.1969260	C	0.8027770	2.5447730	0.6956930
C	2.7426160	-0.6217470	-0.3762210	C	1.8807030	-0.9803580	-0.3363210
C	4.0218910	-0.1255490	-0.6962470	C	3.1261780	-1.0464180	0.3084940
C	4.9034690	-0.8829860	-1.4636680	C	4.0542950	-2.0312190	-0.0308740
C	4.5214520	-2.1424290	-1.9350960	C	3.7600510	-2.9603690	-1.0316460

C	3.2506340	-2.6400620	-1.6344610	C	2.5363410	-2.8861930	-1.6972040
C	2.3648130	-1.8908690	-0.8625790	C	1.6063670	-1.9010490	-1.3548870
H	-1.5944540	-2.3162410	2.1448330	H	-1.1521710	-1.9078960	-0.4950370
H	1.4100630	-1.4533550	3.1966070	H	0.4207310	-0.2045230	3.4835900
H	2.7199510	-1.6353660	2.0048550	H	1.7672460	0.6097140	2.6770240
H	1.1660940	-2.5021550	1.7727230	H	1.6780770	-1.1729430	2.6751210
H	-3.4627450	-0.7900040	2.1561850	H	-3.4371920	-2.4208200	-0.7578530
H	-5.2664910	0.4413580	0.9756120	H	-5.7596620	-1.6992270	-1.2325420
H	-3.5724770	-0.7333200	-2.8138100	H	-6.3355770	0.7213170	-1.2310780
H	-1.7790460	-1.9833620	-1.6089780	H	-4.5739710	2.4095260	-0.7484420
H	1.9450210	1.4204020	-1.9800000	H	-2.2514740	1.6790160	-0.2673670
H	1.7547570	3.8398030	-2.4364550	H	2.7479830	1.0641360	-1.6663990
H	1.3438640	5.4347880	-0.5712030	H	3.4482540	3.4082360	-1.9994970
H	1.1188060	4.5841830	1.7555610	H	2.4710500	5.2171040	-0.5973830
H	1.3176830	2.1657170	2.2168070	H	0.7667260	4.6523070	1.1270040
H	4.3253380	0.8482420	-0.3245670	H	0.0540280	2.2969360	1.4411110
H	5.8906620	-0.4913040	-1.6919420	H	3.3870520	-0.3140940	1.0661740
H	5.2083090	-2.7293770	-2.5383370	H	5.0115210	-2.0656660	0.4822640
H	2.9429170	-3.6113050	-2.0116920	H	4.4837080	-3.7260200	-1.2973000
H	1.3687530	-2.2705180	-0.6523980	H	2.3028280	-3.5901300	-2.4914580
C	-5.5656320	0.6456640	-1.6779180	H	0.6708520	-1.8331250	-1.8982620
N	-6.4085000	1.2241180	-2.2351510				
Molecule 13b				Molecule 13c			
E = -1218.75559623, H (0K) = -1218.368167,				E = -1293.96192460, H (0K) = -1293.569279,			
H (298K) = -1218.343951, G (298K) = -1218.424038				H (298K) = -1293.544393, G (298K) = -1293.625900			
au				au			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	1.1366190	0.0973970	0.0695110	C	1.4047940	0.1003710	0.0545380
O	-0.0718370	-0.0441370	-0.6952270	O	0.2043330	-0.0763100	-0.7165170
C	-0.9615270	-0.9601000	-0.0472410	C	-0.6800200	-1.0057430	-0.0759610
C	-0.5003260	-0.9394980	1.4276230	C	-0.1422130	-1.0918570	1.3715830
N	0.6646460	-0.1790320	1.4406570	N	0.9444930	-0.2192910	1.4214610
C	1.5410070	-0.2525960	2.5997190	C	1.8532910	-0.3198650	2.5561330
F	-0.3220130	-2.2404650	1.8860670	F	0.1914500	-2.4112110	1.6710700
F	-1.4428100	-0.4316720	2.3008930	F	-1.0758100	-0.7810620	2.3343720
C	-2.3975210	-0.5709170	-0.2902690	C	-2.1125570	-0.5589740	-0.2132960
C	-3.3546840	-1.5568190	-0.5423660	C	-3.1097590	-1.4838790	-0.5228480
C	-4.6941890	-1.2135640	-0.7375180	C	-4.4507700	-1.1025720	-0.6298290
C	-5.1091420	0.1226290	-0.6984020	C	-4.8016090	0.2378590	-0.4324000
C	-4.1386300	1.1065870	-0.4495670	C	-3.8025040	1.1795720	-0.1303400
C	-2.8034840	0.7690910	-0.2465910	C	-2.4779520	0.7828220	-0.0206520
C	1.5744060	1.5593960	-0.0850840	C	1.7889100	1.5792210	-0.0774600
C	2.4597540	1.9454690	-1.0985410	C	2.5793820	2.0150630	-1.1485790
C	2.7777870	3.2921950	-1.2876960	C	2.8521230	3.3729540	-1.3231980
C	2.2171430	4.2687510	-0.4628330	C	2.3429740	4.3128160	-0.4247820
C	1.3282170	3.8917820	0.5468920	C	1.5500500	3.8866830	0.6429180
C	1.0053700	2.5470890	0.7304620	C	1.2695710	2.5297280	0.8110990
C	2.2017450	-0.9075830	-0.4075080	C	2.5116060	-0.8508620	-0.4379420
C	3.4816960	-0.9219620	0.1694230	C	3.8084680	-0.7732870	0.0940810
C	4.4362860	-1.8557990	-0.2344630	C	4.8035940	-1.6603900	-0.3173490
C	4.1333590	-2.7846940	-1.2328680	C	4.5235890	-2.6336110	-1.2795210
C	2.8734190	-2.7612740	-1.8311250	C	3.2447740	-2.7026690	-1.8327830
C	1.9171750	-1.8271490	-1.4242650	C	2.2481020	-1.8159280	-1.4174170
H	-0.7873500	-1.9815390	-0.4080140	H	-0.5615400	-2.0048940	-0.5124880
H	0.9169680	-0.2496680	3.4970640	H	1.2505330	-0.4016440	3.4640450
H	2.1803300	0.6335420	2.6308890	H	2.4496980	0.5931050	2.6260090
H	2.1701650	-1.1510770	2.6086770	H	2.5248200	-1.1847320	2.4954060
H	-3.0555420	-2.6016140	-0.5854780	H	-2.8463850	-2.5261820	-0.6869870
H	-5.4241070	-1.9962220	-0.9302060	H	-5.1985230	-1.8481730	-0.8730000
H	-4.4362210	2.1522860	-0.4134270	H	-4.0914300	2.2164490	0.0124530
H	-2.0676850	1.5459650	-0.0635000	H	-1.7123720	1.5196540	0.2019140

H	2.9017850	1.1950070	-1.7455950	H	2.9820810	1.2929660	-1.8515530
H	3.4656160	3.5754470	-2.0797350	H	3.4648610	3.6944060	-2.1609930
H	2.4695690	5.3159070	-0.6060520	H	2.5613060	5.3690840	-0.5564820
H	0.8843140	4.6449430	1.1923250	H	1.1468070	4.6103160	1.3462110
H	0.3080850	2.2527360	1.5081810	H	0.6437070	2.1998020	1.6336980
H	3.7471970	-0.1879390	0.9237590	H	4.0527390	-0.0037440	0.8200350
H	5.4202950	-1.8506350	0.2265130	H	5.8002880	-1.5838860	0.1087020
H	4.8774860	-3.5106260	-1.5487650	H	5.2990120	-3.3226560	-1.6027060
H	2.6313750	-3.4652640	-2.6227830	H	3.0192460	-3.4424860	-2.5961570
H	0.9511640	-1.7981350	-1.9151990	H	1.2663130	-1.8596020	-1.8745080
C	-6.5509720	0.5032080	-0.9412060	O	-6.0705060	0.7287700	-0.5164680
H	-6.8796980	1.2860280	-0.2485210	C	-7.1267220	-0.1785040	-0.8194080
H	-6.6919300	0.8938230	-1.9576220	H	-7.2132250	-0.9608650	-0.0556130
H	-7.2172780	-0.3572460	-0.8244510	H	-8.0390920	0.4194910	-0.8307080
				H	-6.9843990	-0.6442860	-1.8021400
Molecule 13d				Molecule 13e			
E = -1639.03365226, H (0K) = -1638.683434, H (298K) = -1638.659813, G (298K) = -1638.738768 au Imaginary frequency = 0.				E = -1271.68468178, H (0K) = -1271.325961, H (298K) = -1271.301963, G (298K) = -1271.380546 au Imaginary frequency = 0.			
C	1.4168170	0.0981500	0.0697900	C	1.2370230	0.1209460	0.0376110
O	0.1867960	-0.0535430	-0.6613760	O	0.1594830	-0.1755180	-0.8774240
C	-0.6648150	-0.9882140	0.0027820	C	-0.6990700	-1.1897360	-0.3637620
C	-0.1803280	-0.9527920	1.4695220	C	-0.1726690	-1.4442290	1.0674990
N	0.9899640	-0.2039230	1.4498760	N	0.7141370	-0.3954290	1.3188170
C	1.8938390	-0.2660540	2.5878200	C	1.5554400	-0.4931080	2.5079620
F	-0.0097410	-2.2465370	1.9450650	F	0.4204280	-2.7029610	1.1316320
F	-1.1082760	-0.4210060	2.3467290	F	-1.1588960	-1.5073690	2.0184150
C	-2.1157350	-0.6314930	-0.2063930	C	-2.1531990	-0.7683790	-0.4209790
C	-3.0696930	-1.6471100	-0.3206490	C	-3.1486480	-1.7541550	-0.4251400
C	-4.4227910	-1.3440140	-0.4781720	C	-4.4935520	-1.4035250	-0.4519830
C	-4.8091050	-0.0065990	-0.5304310	C	-4.8551140	-0.0455160	-0.4845440
C	-3.8753870	1.0247360	-0.4281140	C	-3.8606860	0.9468190	-0.4899760
C	-2.5292990	0.7041350	-0.2623850	C	-2.5183030	0.5812650	-0.4576450
C	1.8252690	1.5689850	-0.0780510	C	1.3850310	1.6460880	0.0590870
C	2.6910710	1.9827070	-1.0973160	C	2.1357480	2.2920110	-0.9324640
C	2.9808060	3.3374880	-1.2748010	C	2.2029270	3.6850400	-0.9771140
C	2.4106330	4.2938590	-0.4331260	C	1.5255750	4.4515240	-0.0261360
C	1.5405190	3.8889900	0.5823000	C	0.7711180	3.8156600	0.9616610
C	1.2463460	2.5364640	0.7548940	C	0.6949510	2.4218540	0.9993090
C	2.4805100	-0.8851330	-0.4515260	C	2.5217680	-0.5989350	-0.4109500
C	3.7740230	-0.8951870	0.0943950	C	3.7510220	-0.3061900	0.2000290
C	4.7288920	-1.8101590	-0.3500010	C	4.9097080	-0.9943210	-0.1615660
C	4.4122990	-2.7236210	-1.3583320	C	4.8614690	-1.9798510	-1.1500420
C	3.1380790	-2.7039170	-1.9255520	C	3.6476820	-2.2645440	-1.7766170
C	2.1814290	-1.7889290	-1.4782400	C	2.4873040	-1.5786300	-1.4103920
H	-0.4758170	-2.0064170	-0.3599160	H	-0.5660490	-2.1169560	-0.9338200
H	1.2916820	-0.2746080	3.4998900	H	0.9193600	-0.7905380	3.3448880
H	2.5202570	0.6296910	2.6062780	H	1.9776940	0.4889410	2.7328340
H	2.5366180	-1.1548100	2.5791680	H	2.3692350	-1.2194330	2.3997180
H	-2.7603400	-2.6885720	-0.2882100	H	-2.8718400	-2.8048110	-0.4088290
H	-5.1604130	-2.1341030	-0.5670100	H	-5.2620470	-2.1692100	-0.4548620
H	-4.1952260	2.0600790	-0.4764140	H	-4.1429790	1.9940220	-0.5207070
H	-1.7924360	1.4968550	-0.1897510	H	-1.7477410	1.3434230	-0.4713090
H	3.1401090	1.2483600	-1.7578150	H	2.6680420	1.7051940	-1.6742290
H	3.6540850	3.6426950	-2.0711270	H	2.7871350	4.1702120	-1.7541840
H	2.6411540	5.3471760	-0.5675910	H	1.5841740	5.5360810	-0.0560580
H	1.0895110	4.6263750	1.2408280	H	0.2382250	4.4030440	1.7044430
H	0.5643170	2.2199120	1.5374940	H	0.0954350	1.9297230	1.7577470
H	4.0497040	-0.1726390	0.8560490	H	3.8115110	0.4750510	0.9518620
H	5.7235950	-1.8021420	0.0872670	H	5.8509530	-0.7530080	0.3246920

H	5.1566420	-3.4347210	-1.7057950	H	5.7640600	-2.5129980	-1.4355980
H	2.8848670	-3.3958610	-2.7242650	H	3.6003700	-3.0178020	-2.5584000
H	1.2034480	-1.7627920	-1.9450950	H	1.5556530	-1.7910840	-1.9219990
Cl	-6.5149410	0.3920860	-0.7393380	C	-6.2389910	0.3262170	-0.5197660
				N	-7.3627130	0.6282030	-0.5476310
TS² 3a+12				TS² 3b+12			
E = -1179.36067279, H (0K) = -1179.005366, H (298K) = -1178.982071, G (298K) = -1179.059140 au				E = -1218.67898664, H (0K) = -1218.296142, H (298K) = -1218.271016, G (298K) = -1218.353089 au			
Imaginary frequency = 1.				Imaginary frequency = 1.			
C	-1.5053190	0.0003260	0.3926800	C	-1.8136580	0.0214160	0.3954620
O	1.5901260	-2.0942290	-0.8333360	O	1.1660600	-2.1468120	-0.8290150
C	2.0045890	-0.9389920	-1.0172040	C	1.6080560	-0.9955610	-1.0065550
C	0.8962040	0.5575870	0.5150280	C	0.6105240	0.4738740	0.5024470
N	-0.2770730	-0.1465220	0.9190990	N	-0.5910200	-0.1780390	0.9161850
C	0.0760760	-1.2929490	1.7861940	C	-0.2800360	-1.3421870	1.7760390
F	0.6434110	1.6378790	-0.2645180	F	0.3987310	1.5814820	-0.2496320
F	1.6016900	1.0071030	1.5975720	F	1.3553900	0.8630500	1.5803980
C	3.3773610	-0.4993670	-0.6369340	C	3.0086480	-0.6110670	-0.6667900
C	3.8465030	0.7665460	-1.0178640	C	3.5255080	0.6324180	-1.0570120
C	5.1447200	1.1620770	-0.6994240	C	4.8452720	0.9724240	-0.7694410
C	5.9869450	0.2934020	0.0018990	C	5.6891330	0.0813670	-0.0887400
C	5.5260590	-0.9719730	0.3812640	C	5.1636990	-1.1617240	0.2990740
C	4.2287950	-1.3675720	0.0613760	C	3.8457880	-1.5066470	0.0124910
C	-2.3444790	-1.1893510	0.1536490	C	-2.7046310	-1.1305990	0.1602310
C	-3.7130920	-1.1781700	0.4895390	C	-4.0702650	-1.0599080	0.5005210
C	-4.5093880	-2.2969000	0.2571650	C	-4.9149800	-2.1426810	0.2688500
C	-3.9588150	-3.4430720	-0.3239510	C	-4.4162160	-3.3102700	-0.3163950
C	-2.6053750	-3.4620050	-0.6713930	C	-3.0659470	-3.3875540	-0.6683820
C	-1.7998860	-2.3487400	-0.4374340	C	-2.2118890	-2.3111400	-0.4347320
C	-2.0147620	1.3371410	0.0645390	C	-2.2697830	1.3786350	0.0714740
C	-1.6770610	2.4541160	0.8584690	C	-1.8933900	2.4775960	0.8728190
C	-2.2039690	3.7114570	0.5777630	C	-2.3719580	3.7551510	0.5969410
C	-3.0734790	3.8842930	-0.5025660	C	-3.2298260	3.9658030	-0.4860060
C	-3.4161940	2.7879790	-1.3002110	C	-3.6106400	2.8873500	-1.2906720
C	-2.8971890	1.5274920	-1.0191350	C	-3.1409170	1.6067450	-1.0139060
H	1.4856500	-0.2647110	-1.7236690	H	1.1104510	-0.3147030	-1.7232910
H	0.6695760	-2.0203760	1.2299410	H	0.3005660	-2.0776660	1.2161770
H	-0.8370040	-1.7457760	2.1655190	H	-1.2092650	-1.7747060	2.1388870
H	0.6625970	-0.8967590	2.6168010	H	0.3064830	-0.9704970	2.6178750
H	3.1845780	1.4409120	-1.5564580	H	2.8830750	1.3389770	-1.5779280
H	5.5015670	2.1442880	-0.9973580	H	5.2296040	1.9426280	-1.0763210
H	6.9997750	0.5999970	0.2491270	H	5.8006880	-1.8664070	0.8295050
H	6.1822160	-1.6490040	0.9219940	H	3.4465010	-2.4732770	0.3049220
H	3.8578510	-2.3501340	0.3371380	H	-4.4600980	-0.1580660	0.9623440
H	-4.1433300	-0.2933970	0.9485320	H	-5.9628300	-2.0766030	0.5478500
H	-5.5600370	-2.2756310	0.5327590	H	-5.0773590	-4.1523790	-0.5010320
H	-4.5821170	-4.3135120	-0.5087930	H	-2.6766450	-4.2873600	-1.1368160
H	-2.1754810	-4.3448700	-1.1365920	H	-1.1662590	-2.3666330	-0.7290540
H	-0.7524660	-2.3612380	-0.7294650	H	-1.2453660	2.3155610	1.7284770
H	-1.0197560	2.3213870	1.7121070	H	-2.0799600	4.5869970	1.2315460
H	-1.9405680	4.5569820	1.2068250	H	-3.6031210	4.9634530	-0.6993320
H	-3.4848680	4.8660880	-0.7193960	H	-4.2716960	3.0460090	-2.1378920
H	-4.0858520	2.9171720	-2.1457190	H	-3.4322610	0.7758770	-1.6480560
H	-3.1591980	0.6832960	-1.6484660	C	7.1295850	0.4373390	0.1936260
				H	7.4870140	-0.0387760	1.1127930
				H	7.7867390	0.1033310	-0.6207380
				H	7.2628650	1.5195530	0.2939380
TS² 3c+12				TS² 3d+12			
E = -1293.88569622, H (0K) = -1293.497414,				E = -1638.95794907, H (0K) = -1638.612007,			

H (298K) = -1293.471696, G (298K) = -1293.554272				H (298K) = -1638.587714, G (298K) = -1638.667345			
au				au			
Imaginary frequency = 1.				Imaginary frequency = 1.			
C	-2.1127430	0.0044090	0.4061010	C	-2.0931330	0.0269190	0.3953930
O	0.8574080	-2.1004410	-0.8424090	O	0.8040210	-2.1389590	-0.8356840
C	1.2683050	-0.9327290	-1.0181890	C	1.2439940	-0.9751860	-0.9827840
C	0.3102700	0.4667640	0.4905520	C	0.3455270	0.4128820	0.5018270
N	-0.8849170	-0.1915210	0.9154350	N	-0.8798200	-0.2102120	0.9146050
C	-0.5584580	-1.3608750	1.7625480	C	-0.5952010	-1.3980830	1.7517270
F	0.0856900	1.5927900	-0.2292240	F	0.1609220	1.5585560	-0.1975070
F	1.0783540	0.8264320	1.5612880	F	1.1128670	0.7296560	1.5860420
C	2.6762180	-0.5319790	-0.7337920	C	2.6717400	-0.6328840	-0.6765520
C	3.1656820	0.7247570	-1.1301660	C	3.2156870	0.6009970	-1.0586170
C	4.4855840	1.0816030	-0.8965360	C	4.5518540	0.9038390	-0.8032980
C	5.3549510	0.1813650	-0.2559180	C	5.3444970	-0.0462820	-0.1583920
C	4.8818980	-1.0778230	0.1428530	C	4.8301590	-1.2841190	0.2296820
C	3.5523080	-1.4203420	-0.1013140	C	3.4927640	-1.5695960	-0.0361780
C	-2.9995840	-1.1507250	0.1713940	C	-3.0221040	-1.0953820	0.1637140
C	-4.3634280	-1.0884550	0.5202400	C	-4.3823910	-0.9809130	0.5118870
C	-5.2040990	-2.1740400	0.2870720	C	-5.2618120	-2.0352390	0.2783920
C	-4.7029340	-3.3353880	-0.3084520	C	-4.8028820	-3.2128240	-0.3191670
C	-3.3543990	-3.4039790	-0.6690680	C	-3.4580380	-3.3312730	-0.6809890
C	-2.5040470	-2.3250810	-0.4337410	C	-2.5683700	-2.2855740	-0.4428210
C	-2.5807690	1.3608670	0.0954150	C	-2.5154650	1.3961570	0.0739980
C	-2.2130590	2.4549520	0.9072030	C	-2.1338340	2.4788740	0.8938440
C	-2.7036640	3.7307510	0.6446700	C	-2.5863270	3.7666950	0.6225990
C	-3.5648530	3.9441830	-0.4351070	C	-3.4194650	4.0016990	-0.4746540
C	-3.9374360	2.8703220	-1.2497140	C	-3.8050470	2.9383800	-1.2969630
C	-3.4562030	1.5912620	-0.9859440	C	-3.3652180	1.6467640	-1.0227980
H	0.7455730	-0.2669060	-1.7325050	H	0.7722290	-0.2959360	-1.7195830
H	0.0375820	-2.0772530	1.1936980	H	-0.0133860	-2.1231080	1.1787820
H	-1.4816250	-1.8146820	2.1142080	H	-1.5337330	-1.8308710	2.0882500
H	0.0169410	-0.9900610	2.6123990	H	-0.0183910	-1.0526160	2.6109770
H	2.4975490	1.4286760	-1.6209130	H	2.5868960	1.3350410	-1.5563710
H	4.8713480	2.0497900	-1.2013420	H	4.9729300	1.8583400	-1.1007750
H	5.5367960	-1.7895110	0.6323740	H	5.4671440	-2.0100930	0.7241000
H	3.1784860	-2.3969170	0.1915710	H	3.0688270	-2.5297890	0.2404740
H	-4.7548770	-0.1913100	0.9897560	H	-4.7404640	-0.0701160	0.9816300
H	-6.2505600	-2.1150330	0.5727370	H	-6.3053220	-1.9388180	0.5641880
H	-5.3610430	-4.1796010	-0.4943570	H	-5.4916090	-4.0319270	-0.5062050
H	-2.9637500	-4.2990110	-1.1454590	H	-3.1012570	-4.2391410	-1.1593220
H	-1.4593710	-2.3724510	-0.7337940	H	-1.5258160	-2.3691220	-0.7419380
H	-1.5627450	2.2900500	1.7605530	H	-1.5044040	2.2964300	1.7590970
H	-2.4184490	4.5589330	1.2870800	H	-2.2929580	4.5873320	1.2708000
H	-3.9472390	4.9405090	-0.6382400	H	-3.7710790	5.0077130	-0.6852520
H	-4.6012570	3.0313740	-2.0942990	H	-4.4478570	3.1170920	-2.1539980
H	-3.7413590	0.7638030	-1.6273330	H	-3.6614870	0.8260230	-1.6677160
O	6.6315170	0.6220290	-0.0730390	Cl	7.0400350	0.3233950	0.1670690
C	7.5626350	-0.2457460	0.5680550				
H	8.5038950	0.3044180	0.6072690				
H	7.2424730	-0.4930860	1.5874330				
H	7.7051840	-1.1712380	-0.0028460				
TS² 3e+12				Molecule 15a			
E = -1271.60814288, H (0K) = -1271.254324,				E = -1179.37072020, H (0K) = -1179.013154,			
H (298K) = -1271.229163, G (298K) = -1271.310925				H (298K) = -1178.990502, G (298K) = -1179.065104			
au				au			
Imaginary frequency = 1.				Imaginary frequency = 0.			
C	-1.9744940	0.0396600	0.3951420	C	-1.4360260	-0.0010960	0.4730360
O	1.0109080	-2.2236480	-0.9561780	O	1.2683890	-2.1202330	-0.3010260
C	1.4685220	-1.0910680	-1.1544270	C	1.5302540	-0.8241630	-0.3589030
C	0.4494250	0.5144310	0.4226560	C	0.9924730	0.0091060	0.9278490

N	-0.7337470	-0.1494620	0.8732020	N	-0.3970810	-0.4165400	1.2044360
C	-0.3884430	-1.3013360	1.7363850	C	-0.4151470	-1.6718610	1.9876570
F	0.2033260	1.5821420	-0.3765270	F	1.0648000	1.3419430	0.6889680
F	1.1892970	0.9734330	1.4787420	F	1.7276800	-0.2251240	2.0454680
C	2.8534760	-0.6992110	-0.7604310	C	3.0223570	-0.4564190	-0.5115070
C	3.3725000	0.5498360	-1.1344530	C	3.4442440	0.7572310	-1.0682500
C	4.6753400	0.9007240	-0.8054670	C	4.8051400	1.0396910	-1.2128610
C	5.4800460	-0.0086090	-0.0934110	C	5.7611130	0.1107660	-0.7940710
C	4.9675910	-1.2652940	0.2802860	C	5.3468510	-1.1036680	-0.2376300
C	3.6637120	-1.6031300	-0.0573980	C	3.9867500	-1.3830680	-0.1017410
C	-2.8687410	-1.1181820	0.2056800	C	-2.4556230	-0.9678590	0.0354370
C	-4.2196580	-1.0491630	0.6005830	C	-3.8276520	-0.6573070	0.0971390
C	-5.0683670	-2.1375790	0.4147140	C	-4.7691600	-1.5665970	-0.3766670
C	-4.5890960	-3.3089140	-0.1790940	C	-4.3508970	-2.7749340	-0.9430470
C	-3.2542380	-3.3846040	-0.5857160	C	-2.9882220	-3.0785790	-1.0289270
C	-2.3962060	-2.3026680	-0.3970580	C	-2.0371030	-2.1905840	-0.5339600
C	-2.4455040	1.3914850	0.0723070	C	-1.6155870	1.4159790	0.1290110
C	-2.0320000	2.5016800	0.8393740	C	-1.3776620	2.4186630	1.0919450
C	-2.5230220	3.7750930	0.5670990	C	-1.6442100	3.7517600	0.7967020
C	-3.4297970	3.9699090	-0.4783930	C	-2.1337330	4.1069790	-0.4635110
C	-3.8468550	2.8803590	-1.2493910	C	-2.3737940	3.1213050	-1.4262070
C	-3.3647780	1.6037050	-0.9759090	C	-2.1335580	1.7835980	-1.1294870
H	0.9717790	-0.3933330	-1.8519980	H	0.9623250	-0.2582260	-1.1514000
H	0.1415440	-2.0635200	1.1633500	H	0.2407330	-2.3873890	1.4790730
H	-1.3001050	-1.7068730	2.1691540	H	-1.4357000	-2.0373820	2.0620770
H	0.2578330	-0.9224750	2.5298650	H	-0.0293100	-1.4368090	2.9806760
H	2.7437990	1.2512290	-1.6763700	H	2.7048700	1.4832090	-1.3987420
H	5.0770040	1.8668460	-1.0927420	H	5.1186510	1.9821520	-1.6555900
H	5.5960390	-1.9627090	0.8246440	H	6.8203220	0.3280580	-0.9071050
H	3.2541340	-2.5713580	0.2110380	H	6.0861110	-1.8335190	0.0844560
H	-4.5940240	-0.1442690	1.0690300	H	3.6394540	-2.3287480	0.3027000
H	-6.1040990	-2.0726970	0.7357970	H	-4.1486450	0.2828610	0.5342360
H	-5.2535820	-4.1553330	-0.3282630	H	-5.8273210	-1.3325770	-0.3091690
H	-2.8805380	-4.2871890	-1.0612410	H	-5.0875380	-3.4778000	-1.3219280
H	-1.3646900	-2.3599280	-0.7352800	H	-2.6667000	-4.0097130	-1.4864330
H	-1.3442660	2.3520130	1.6657730	H	-0.9681060	-2.4000640	-0.6082960
H	-2.2024570	4.6160850	1.1751960	H	-1.0166910	2.1399720	2.0759940
H	-3.8128450	4.9644630	-0.6887290	H	-1.4732310	4.5141280	1.5507110
H	-4.5459000	3.0272510	-2.0676650	H	-2.3346400	5.1494860	-0.6928820
H	-3.6845270	0.7639340	-1.5840220	H	-2.7513600	3.3960050	-2.4064170
C	6.8253670	0.3445690	0.2486620	H	-2.3179380	1.0189770	-1.8767640
N	7.9187970	0.6318470	0.5270130				
Molecule 15b				Molecule 15c			
E = -1218.68850177, H (0K) = -1218.303531, H (298K) = -1218.278970, G (298K) = -1218.358562 au.				E = -1293.89467182, H (0K) = -1293.504433, H (298K) = -1293.479172, G (298K) = -1293.559729 au			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	-1.7622670	0.0109090	0.4624050	C	-2.0698850	-0.0087870	0.4601870
O	0.9202600	-2.1569350	-0.2387430	O	0.6666880	-2.1139120	-0.2145110
C	1.2085860	-0.8657660	-0.2814690	C	0.9239430	-0.8162020	-0.2616700
C	0.6492280	-0.0308250	0.9960640	C	0.3374140	0.0072470	1.0120050
N	-0.7567870	-0.4288160	1.2258670	N	-1.0604040	-0.4221350	1.2332480
C	-0.8260630	-1.6873400	2.0009900	C	-1.1070510	-1.6786670	2.0133330
F	0.7566880	1.3021310	0.7713240	F	0.4157680	1.3424320	0.7865700
F	1.3445700	-0.2897030	2.1335260	F	1.0311170	-0.2344950	2.1541490
C	2.7092920	-0.5253890	-0.3906130	C	2.4141410	-0.4381810	-0.3664190
C	3.1753520	0.6828530	-0.9205540	C	2.8545370	0.7877080	-0.8872880
C	4.5448410	0.9386800	-1.0199090	C	4.2108420	1.0814190	-0.9854450
C	5.4896470	-0.0024840	-0.5893500	C	5.1655760	0.1480430	-0.5531630
C	5.0150210	-1.2108990	-0.0559400	C	4.7424420	-1.0817370	-0.0316110
C	3.6486790	-1.4688980	0.0372800	C	3.3755910	-1.3582680	0.0524110

C	-2.7864850	-0.9326420	-0.0137220	C	-3.0683210	-0.9777080	-0.0200430
C	-4.1531120	-0.5937900	0.0027330	C	-4.4425070	-0.6705600	-0.0158720
C	-5.0965820	-1.4813140	-0.5071060	C	-5.3611310	-1.5817800	-0.5293390
C	-4.6845240	-2.6959680	-1.0644930	C	-4.9167140	-2.7889490	-1.0780350
C	-3.3263290	-3.0277000	-1.1052290	C	-3.5509450	-3.0893780	-1.1064160
C	-2.3744670	-2.1616300	-0.5741010	C	-2.6236550	-2.1992570	-0.5715500
C	-1.9013920	1.4330930	0.1196290	C	-2.2398610	1.4086930	0.1114740
C	-1.6773780	2.4265830	1.0952570	C	-2.0468850	2.4103060	1.0853940
C	-1.9064210	3.7661530	0.7975800	C	-2.3053030	3.7431710	0.7816200
C	-2.3441250	4.1367650	-0.4771480	C	-2.7422060	4.0993790	-0.4974660
C	-2.5700230	3.1602790	-1.4525490	C	-2.9376430	3.1147030	-1.4712210
C	-2.3673060	1.8166930	-1.1543160	C	-2.7052470	1.7772530	-1.1670860
H	0.6715230	-0.2840490	-1.0844980	H	0.3731350	-0.2505270	-1.0673930
H	-0.1683070	-2.4139380	1.5108640	H	-0.4287430	-2.3919300	1.5319930
H	-1.8556970	-2.0323780	2.0398720	H	-2.1287170	-2.0473170	2.0450490
H	-0.4686840	-1.4652020	3.0075640	H	-0.7636180	-1.4441470	3.0219720
H	2.4645150	1.4316580	-1.2629140	H	2.1279870	1.5211820	-1.2290350
H	4.8852990	1.8830870	-1.4404650	H	4.5545740	2.0258950	-1.3978200
H	5.7286910	-1.9584980	0.2862550	H	5.4605060	-1.8229930	0.3015010
H	3.2781790	-2.4120840	0.4269180	H	3.0287740	-2.3150410	0.4304850
H	-4.4693010	0.3512170	0.4328620	H	-4.7839080	0.2687380	0.4074400
H	-6.1513420	-1.2254230	-0.4746700	H	-6.4217550	-1.3502020	-0.5064890
H	-5.4222950	-3.3817130	-1.4715240	H	-5.6351780	-3.4932890	-1.4878520
H	-3.0087040	-3.9635620	-1.5557820	H	-3.2082110	-4.0196060	-1.5502200
H	-1.3080650	-2.3927150	-0.6130940	H	-1.5518910	-2.4057080	-0.6008560
H	-1.3568890	2.1363400	2.0899360	H	-1.7267980	2.1308250	2.0832740
H	-1.7466240	4.5215900	1.5609800	H	-2.1690080	4.5045590	1.5436760
H	-2.5158160	5.1841100	-0.7082070	H	-2.9368640	5.1416410	-0.7332740
H	-2.9072510	3.4468130	-2.4440310	H	-3.2741850	3.3900180	-2.4661160
H	-2.5407150	1.0591930	-1.9114200	H	-2.8550110	1.0135240	-1.9229920
C	6.9723160	0.2599040	-0.7239490	O	6.4734470	0.5274390	-0.6894210
H	7.5344250	-0.1813390	0.1066780	C	7.4829630	-0.3829610	-0.2691970
H	7.3731920	-0.1745050	-1.6499110	H	8.4348140	0.1145570	-0.4630190
H	7.1890460	1.3331320	-0.7491300	H	7.4020860	-0.6071800	0.8018540
				H	7.4412250	-1.3206280	-0.8375380
Molecule 15d				Molecule 15e			
E = -1638.96863098, H (0K) = -1638.620758,				E = -1271.62091455, H (0K) = -1271.264694			
H (298K) = -1638.596834, G (298K) = -1638.674942				H (298K) = -1271.240204, G (298K) = -1271.319361			
au.				au.			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	-2.0615770	0.0153640	0.4533970	C	-1.9390650	0.0151110	0.4519910
O	0.6247330	-2.1529750	-0.2251450	O	0.7535970	-2.1449550	-0.2507170
C	0.9197850	-0.8637620	-0.2529550	C	1.0439670	-0.8556680	-0.2771940
C	0.3442090	-0.0333550	1.0161300	C	0.4729680	-0.0250490	0.9916860
N	-1.0657380	-0.4298380	1.2256210	N	-0.9333940	-0.4280750	1.2124130
C	-1.1493840	-1.6880790	2.0011120	C	-1.0063750	-1.6855610	1.9912160
F	0.4582060	1.3004840	0.7974650	F	0.5802310	1.3085350	0.7685030
F	1.0233350	-0.2980880	2.1617420	F	1.1620110	-0.2844280	2.1326010
C	2.4290170	-0.5405020	-0.3258780	C	2.5550860	-0.5324040	-0.3501960
C	2.9241030	0.6782580	-0.8034840	C	3.0488200	0.6894640	-0.8260550
C	4.2980470	0.9177840	-0.8782870	C	4.4188970	0.9223040	-0.9046970
C	5.1765760	-0.0802380	-0.4607370	C	5.3183150	-0.0784020	-0.4958950
C	4.7125310	-1.3056180	0.0173630	C	4.8302250	-1.3094500	-0.0188290
C	3.3367760	-1.5242740	0.0764970	C	3.4588540	-1.5250990	0.0442940
C	-3.0859200	-0.9228090	-0.0317510	C	-2.9663030	-0.9253660	-0.0212140
C	-4.4508040	-0.5764620	-0.0282480	C	-4.3317530	-0.5813990	-0.0032810
C	-5.3937660	-1.4592980	-0.5468510	C	-5.2783860	-1.4662820	-0.5113870
C	-4.9823700	-2.6757620	-1.1008400	C	-4.8704180	-2.6819920	-1.0695620
C	-3.6255620	-3.0144750	-1.1294160	C	-3.5133460	-3.0182210	-1.1128140
C	-2.6745610	-2.1536510	-0.5886480	C	-2.5583980	-2.1556190	-0.5822330
C	-2.1902430	1.4373920	0.1070270	C	-2.0747840	1.4361960	0.1060820

C	-1.9752200	2.4311980	1.0844410	C	-1.8526000	2.4310580	1.0809770
C	-2.1967890	3.7708880	0.7820800	C	-2.0818770	3.7696980	0.7802050
C	-2.6167870	4.1408380	-0.4988300	C	-2.5159330	4.1373610	-0.4967330
C	-2.8332670	3.1639560	-1.4759760	C	-2.7392460	3.1594440	-1.4713140
C	-2.6392410	1.8201520	-1.1732850	C	-2.5383430	1.8164260	-1.1698670
H	0.4122020	-0.2734840	-1.0676940	H	0.5421680	-0.2657900	-1.0949420
H	-0.4892280	-2.4182010	1.5206550	H	-0.3490370	-2.4152300	1.5069550
H	-2.1808400	-2.0285340	2.0276200	H	-2.0366910	-2.0283570	2.0277250
H	-0.8039380	-1.4660520	3.0118170	H	-0.6527240	-1.4602210	2.9983170
H	2.2354070	1.4530610	-1.1300430	H	2.3581530	1.4647840	-1.1454020
H	4.6786480	1.8607430	-1.2572600	H	4.7979900	1.8672830	-1.2811540
H	5.4141100	-2.0723350	0.3304250	H	5.5283060	-2.0813260	0.2904800
H	2.9336990	-2.4730730	0.4159960	H	3.0481290	-2.4720110	0.3785840
H	-4.7661100	0.3699330	0.3993820	H	-4.6442800	0.3643130	0.4278110
H	-6.4474950	-1.1983730	-0.5240880	H	-6.3323090	-1.2075500	-0.4773220
H	-5.7197180	-3.3576430	-1.5149880	H	-5.6107960	-3.3653610	-1.4757060
H	-3.3084980	-3.9515500	-1.5777020	H	-3.1993270	-3.9546240	-1.5645220
H	-1.6092320	-2.3896770	-0.6184400	H	-1.4933060	-2.3898060	-0.6240000
H	-1.6685390	2.1413640	2.0835600	H	-1.5350900	2.1427840	2.0771500
H	-2.0448970	4.5269290	1.5464280	H	-1.9250560	4.5267120	1.5425390
H	-2.7822960	5.1883660	-0.7334290	H	-2.6872230	5.1842100	-0.7301340
H	-3.1568970	3.4503260	-2.4719770	H	-3.0738880	3.4443760	-2.4640420
H	-2.8060010	1.0620130	-1.9312110	H	-2.7107110	1.0572540	-1.9254730
Cl	6.9202800	0.2095320	-0.5516050	C	6.7296120	0.1529610	-0.5727300
				N	7.8772860	0.3415300	-0.6332370
TS³ (3a)				TS³ (3b)			
E = -1179.36537114, H (0K) = -1179.008280,				E = -1218.68302367, H (0K) = -1218.298612,			
H (298K) = -1178.986131, G (298K) = -1179.059521				H (298K) = -1218.274483, G (298K) = -1218.353299			
au				au			
Imaginary frequency = 1.				Imaginary frequency = 1.			
C	-1.3646990	-0.0289950	0.4805590	C	-1.6891490	-0.0400200	0.4726610
O	0.8404430	-1.3494790	-0.9830090	O	0.5693990	-1.3150120	-0.9370970
C	1.4437420	-0.2675850	-0.5164180	C	1.1421310	-0.2210520	-0.4585920
C	1.0252770	0.0695390	1.0145410	C	0.6841230	0.1076080	1.0628720
N	-0.3610060	-0.4328190	1.2497730	N	-0.6971430	-0.4209980	1.2681160
C	-0.3786390	-1.7684700	1.8848390	C	-0.7037170	-1.7556460	1.9053270
F	1.1208620	1.4000620	1.2837450	F	0.7476020	1.4399320	1.3336820
F	1.8157520	-0.5451190	1.9332580	F	1.4657460	-0.4912890	1.9993760
C	2.9908130	-0.2980030	-0.5244520	C	2.6880270	-0.2217050	-0.4353270
C	3.7614700	0.8623720	-0.3781240	C	3.4393010	0.9470910	-0.2638150
C	5.1564670	0.8000630	-0.4195100	C	4.8346000	0.9066400	-0.2746200
C	5.7977050	-0.4275650	-0.6085790	C	5.5225890	-0.3012620	-0.4605710
C	5.0334930	-1.5884740	-0.7596290	C	4.7624530	-1.4672090	-0.6321040
C	3.6396610	-1.5199610	-0.7197690	C	3.3679040	-1.4266760	-0.6234050
C	-2.4712570	-0.9401990	0.1168500	C	-2.7704840	-0.9735230	0.0891440
C	-3.8018070	-0.5741430	0.3875850	C	-4.1128210	-0.6351200	0.3360880
C	-4.8442570	-1.4196510	0.0147350	C	-5.1305900	-1.5025340	-0.0544110
C	-4.5702260	-2.6094460	-0.6659390	C	-4.8197650	-2.6867400	-0.7289980
C	-3.2506020	-2.9574130	-0.9701590	C	-3.4879890	-3.0071530	-1.0095350
C	-2.1975740	-2.1347160	-0.5775200	C	-2.4595170	-2.1622480	-0.5991230
C	-1.4942510	1.3711960	0.0367770	C	-1.8346410	1.3553660	0.0184570
C	-1.3625080	2.4378250	0.9464180	C	-1.7467650	2.4288030	0.9252130
C	-1.6028400	3.7441780	0.5278450	C	-2.0015570	3.7281850	0.4934860
C	-1.9531780	4.0033740	-0.7993220	C	-2.3229500	3.9738890	-0.8435080
C	-2.0884660	2.9490590	-1.7084780	C	-2.4146150	2.9125310	-1.7499320
C	-1.8855350	1.6383450	-1.2896570	C	-2.1970230	1.6081610	-1.3188440
H	1.1527510	0.6973520	-1.0142300	H	0.8417290	0.7377930	-0.9626030
H	0.1738590	-2.4614630	1.2467500	H	-0.1258500	-2.4393150	1.2796730
H	-1.4085670	-2.0928470	2.0049000	H	-1.7298770	-2.0985010	2.0046990
H	0.1001990	-1.6878000	2.8590150	H	-0.2465830	-1.6650640	2.8889770
H	3.2681250	1.8213930	-0.2343730	H	2.9316250	1.8985480	-0.1186500

H	5.7427530	1.7093970	-0.3091160	H	5.3993440	1.8274960	-0.1397280
H	6.8831290	-0.4771540	-0.6459960	H	5.2725730	-2.4178630	-0.7792290
H	5.5259560	-2.5459020	-0.9150010	H	2.7713650	-2.3211690	-0.7746060
H	3.0191700	-2.4005150	-0.8551410	H	-4.3517030	0.2907280	0.8504080
H	-4.0120880	0.3561160	0.9063150	H	-6.1650650	-1.2498000	0.1579310
H	-5.8692940	-1.1455300	0.2454520	H	-5.6165480	-3.3535010	-1.0463730
H	-5.3862580	-3.2590600	-0.9696530	H	-3.2502970	-3.9143240	-1.5574960
H	-3.0416840	-3.8687310	-1.5229220	H	-1.4168130	-2.3532570	-0.8364410
H	-1.1637990	-2.3478060	-0.8340010	H	-1.5083670	2.2370440	1.9647260
H	-1.1018290	2.2358260	1.9786140	H	-1.9492600	4.5488700	1.2025120
H	-1.5167440	4.5597780	1.2394150	H	-2.5110540	4.9900670	-1.1778730
H	-2.1299260	5.0248270	-1.1236420	H	-2.6649820	3.1016190	-2.7892930
H	-2.3614320	3.1487240	-2.7401360	H	-2.2745940	0.7806460	-2.0162800
H	-1.9970730	0.8164970	-1.9891810	C	7.0333170	-0.3386680	-0.5084940
				H	7.4202220	-1.3104920	-0.1831780
				H	7.4070190	-0.1665600	-1.5272000
				H	7.4746400	0.4340230	0.1306440
TS³ (3c)				TS³ (3d)			
E = -1293.88904866, H (0K) = -1293.499293,				E = -1638.96347341, H (0K) = -1638.616120,			
H (298K) = -1293.474501, G (298K) = -1293.554107				H (298K) = -1638.592659, G (298K) = -1638.669767			
au				au			
Imaginary frequency = 1.				Imaginary frequency = 1.			
C	-1.9917810	-0.0704260	0.4654810	C	-1.9900170	-0.0449290	0.4717820
O	0.3586600	-1.2356340	-0.8807230	O	0.3041490	-1.3020200	-0.9080900
C	0.8673320	-0.1036400	-0.4189810	C	0.8497340	-0.1995900	-0.4187210
C	0.3585940	0.2416950	1.0854580	C	0.3746890	0.1073690	1.0959390
N	-0.9890780	-0.3682580	1.2831810	N	-1.0083550	-0.4261700	1.2795380
C	-0.9173870	-1.6871040	1.9488310	C	-1.0290320	-1.7526210	1.9340090
F	0.3313760	1.5839710	1.3099810	F	0.4349100	1.4349950	1.3910310
F	1.1577610	-0.2723170	2.0570050	F	1.1480260	-0.5083250	2.0281660
C	2.4095030	-0.0296210	-0.3669150	C	2.3967270	-0.1793240	-0.3800470
C	3.1056720	1.1731390	-0.1743450	C	3.1323510	0.9958020	-0.1873230
C	4.4963800	1.2033990	-0.1614160	C	4.5285670	0.9792520	-0.1901430
C	5.2276910	0.0191810	-0.3442340	C	5.1846570	-0.2346990	-0.3893050
C	4.5470470	-1.1880960	-0.5440320	C	4.4778450	-1.4197280	-0.5890600
C	3.1485920	-1.1956720	-0.5541830	C	3.0832910	-1.3777860	-0.5845840
C	-3.0050030	-1.0803020	0.0884600	C	-3.0627170	-0.9801620	0.0724290
C	-4.3697840	-0.8220960	0.3084200	C	-4.4107390	-0.6387560	0.2818470
C	-5.3251280	-1.7606340	-0.0751940	C	-5.4183440	-1.5096800	-0.1263740
C	-4.9304000	-2.9381970	-0.7166400	C	-5.0906640	-2.6998130	-0.7823400
C	-3.5769370	-3.1803280	-0.9704610	C	-3.7523600	-3.0230190	-1.0267640
C	-2.6098520	-2.2629370	-0.5663750	C	-2.7345140	-2.1751230	-0.5972320
C	-2.2222420	1.3027770	-0.0201260	C	-2.1261610	1.3488940	0.0115880
C	-2.2157830	2.3981120	0.8644090	C	-2.0493930	2.4244020	0.9170910
C	-2.5493120	3.6689520	0.4025170	C	-2.2955380	3.7229700	0.4782490
C	-2.8699500	3.8656540	-0.9427500	C	-2.5962430	3.9655840	-0.8641270
C	-2.8815620	2.7821510	-1.8272260	C	-2.6765190	2.9021970	-1.7693300
C	-2.5845040	1.5039320	-1.3662060	C	-2.4683570	1.5985460	-1.3317930
H	0.5283900	0.8264710	-0.9520600	H	0.5459640	0.7566060	-0.9248990
H	-0.2829020	-2.3421050	1.3477110	H	-0.4405470	-2.4478330	1.3319410
H	-1.9194850	-2.0973020	2.0374290	H	-2.0576960	-2.0918300	2.0185660
H	-0.4860550	-1.5455620	2.9381140	H	-0.5911600	-1.6487930	2.9252420
H	2.5543460	2.1004580	-0.0341450	H	2.6157360	1.9403790	-0.0349530
H	5.0385100	2.1337880	-0.0166740	H	5.0964690	1.8925230	-0.0445530
H	5.0890270	-2.1147590	-0.6988010	H	5.0083910	-2.3528200	-0.7509120
H	2.5967990	-2.1146920	-0.7271380	H	2.4903680	-2.2703110	-0.7570080
H	-4.6743830	0.0983930	0.7969120	H	-4.6623140	0.2916810	0.7814640
H	-6.3765440	-1.5686910	0.1166390	H	-6.4577880	-1.2551500	0.0573570
H	-5.6787560	-3.6610710	-1.0290290	H	-5.8793460	-3.3692790	-1.1138240
H	-3.2743150	-4.0832970	-1.4927730	H	-3.5013990	-3.9345690	-1.5612530
H	-1.5538270	-2.3944760	-0.7839580	H	-1.6866970	-2.3684420	-0.8085270

H	-1.9783430	2.2437110	1.9103660	H	-1.8276460	2.2349500	1.9606360
H	-2.5591420	4.5056670	1.0944670	H	-2.2527570	4.5453690	1.1858620
H	-3.1198220	4.8602760	-1.3006530	H	-2.7773000	4.9812380	-1.2038550
H	-3.1314940	2.9330740	-2.8729170	H	-2.9108880	3.0892740	-2.8127290
H	-2.5999600	0.6589980	-2.0465080	H	-2.5368770	0.7693690	-2.0281350
O	6.5911010	0.1516940	-0.3196030	Cl	6.9553400	-0.2683380	-0.4023520
C	7.3797050	-1.0177120	-0.5022580				
H	8.4194970	-0.6910540	-0.4436160				
H	7.1877910	-1.7598510	0.2830640				
H	7.1985460	-1.4768860	-1.4823660				
TS³ (3e)				Molecule 16			
E = -1271.61610765, H (0K) = -1271.260419, H (298K) = -1271.236403, G (298K) = -1271.314557 au Imaginary frequency = 1.				E = -1061.64809906, H (0K) = -1061.361680, H (298K) = -1061.340913, G (298K) = -1061.412097 au Imaginary frequency = 0.			
C	-1.8685140	-0.0437170	0.4730580	C	0.5159700	0.1403160	0.2602020
O	0.4203260	-1.3135850	-0.9218110	C	-0.8695440	-1.1626020	1.8363620
C	0.9666020	-0.2142270	-0.4295780	N	-0.6644660	-0.1790980	0.8515220
C	0.5007430	0.0854740	1.0869030	C	-1.8831930	0.5948990	0.5886300
N	-0.8852330	-0.4389380	1.2721270	F	-1.9850270	-1.9197140	1.5905950
C	-0.9178050	-1.7635680	1.9305370	F	0.1677660	-2.0050070	2.0154820
F	0.5742550	1.4092030	1.3950020	C	1.4366190	-0.9276140	-0.1330520
F	1.2747640	-0.5469340	2.0074150	C	2.8360020	-0.7419520	-0.0922820
C	2.5145340	-0.1964470	-0.3954520	C	3.7026020	-1.7525030	-0.4973940
C	3.2514420	0.9800920	-0.2030440	C	3.1979350	-2.9761140	-0.9505310
C	4.6425330	0.9589160	-0.2161740	C	1.8160570	-3.1777200	-0.9958050
C	5.3174250	-0.2578780	-0.4251900	C	0.9439600	-2.1697500	-0.5929160
C	4.5836050	-1.4422370	-0.6234930	C	0.8865390	1.5591170	0.1253770
C	3.1941360	-1.3990520	-0.6106280	C	1.5508230	2.0320050	-1.0252850
C	-2.9507530	-0.9674890	0.0754480	C	1.9007580	3.3744670	-1.1459160
C	-4.2952860	-0.6113730	0.2833820	C	1.5973350	4.2798570	-0.1239670
C	-5.3114800	-1.4720690	-0.1248890	C	0.9444820	3.8266600	1.0249860
C	-4.9955910	-2.6659490	-0.7799040	C	0.5961470	2.4828610	1.1515090
C	-3.6606000	-3.0035270	-1.0233280	H	-2.4810890	0.6604410	1.4999630
C	-2.6343540	-2.1664690	-0.5929900	H	-1.6231790	1.6087600	0.2844980
C	-1.9919640	1.3521870	0.0168250	H	3.2391920	0.1966080	0.2741880
C	-1.8987320	2.4249330	0.9242970	H	4.7759980	-1.5898110	-0.4508460
C	-2.1336320	3.7267940	0.4893760	H	3.8763850	-3.7629530	-1.2684330
C	-2.4386690	3.9752770	-0.8509870	H	1.4147030	-4.1214280	-1.3552830
C	-2.5351560	2.9148340	-1.7580600	H	-0.1288070	-2.3140940	-0.6681600
C	-2.3389740	1.6081150	-1.3243350	H	1.7775880	1.3397190	-1.8302840
H	0.6688060	0.7450190	-0.9334010	H	2.4051120	3.7179300	-2.0450580
H	-0.3384150	-2.4677660	1.3303640	H	1.8700320	5.3268210	-0.2216480
H	-1.9498590	-2.0911500	2.0190440	H	0.7168910	4.5180400	1.8318650
H	-0.4764170	-1.6609900	2.9203870	H	0.1172830	2.1334720	2.0625330
H	2.7340090	1.9225440	-0.0442750	C	-2.7029300	-0.0511450	-0.5263400
H	5.2107900	1.8723050	-0.0700620	O	-2.3182700	-0.9168090	-1.2815380
H	5.1083930	-2.3781220	-0.7902470	O	-3.9172280	0.5141610	-0.5640420
H	2.5930790	-2.2856870	-0.7827840	C	-4.8018320	0.0456970	-1.6051770
H	-4.5372390	0.3220150	0.7821940	H	-4.9931400	-1.0228380	-1.4849220
H	-6.3483500	-1.2067410	0.0578740	H	-5.7211320	0.6166860	-1.4820400
H	-5.7909780	-3.3272990	-1.1115750	H	-4.3616220	0.2311410	-2.5874790
H	-3.4189320	-3.9177530	-1.5574400				
H	-1.5888350	-2.3715590	-0.8043080				
H	-1.6740900	2.2311130	1.9663760				
H	-2.0787970	4.5471930	1.1984270				
H	-2.6106740	4.9935030	-1.1876420				
H	-2.7730870	3.1066690	-2.7997550				
H	-2.4203570	0.7812500	-2.0220180				
C	6.7489080	-0.2883910	-0.4434540				
N	7.9133260	-0.3141560	-0.4561750				

TS ⁴				TS ⁵			
E = -1407.23077911, H (0K) = -1406.832799, H (298K) = -1406.804870, G (298K) = -1406.894023 au				E = -1407.23299921, H (0K) = -1406.834702, H (298K) = -1406.806964, G (298K) = -1406.895033 au			
Imaginary frequency = 1.				Imaginary frequency = 1.			
C	-1.2578380	0.4512910	-0.0182850	C	-1.5628910	0.1465550	-0.0825980
O	1.2832500	0.5013470	2.3383570	O	1.5473780	-1.2171500	-2.0850590
C	2.0036890	-0.3385130	1.7846130	C	1.8778820	-0.0514980	-1.8090010
C	0.9825140	-0.5193390	-0.4087630	C	0.8563640	0.5508650	0.2347160
N	-0.4073050	-0.5907470	-0.1197330	N	-0.3236120	-0.2457590	0.2792500
C	-0.8116860	-1.9508870	0.2610140	C	-0.0001090	-1.6500650	0.5713780
F	1.3718470	-1.5556120	-1.2154800	F	0.6200480	1.8764770	0.1271260
F	1.3573680	0.6287460	-1.0036680	F	1.6248920	0.3571430	1.3476830
C	3.3443080	-0.0261320	1.2176900	C	3.2530310	0.3161830	-1.3635280
C	4.1806310	-1.0606400	0.7749830	C	3.6267870	1.6637440	-1.2538170
C	5.4493110	-0.7740370	0.2726240	C	4.9228240	2.0064770	-0.8709480
C	5.8901000	0.5513890	0.2084470	C	5.8575000	1.0036010	-0.5953320
C	5.0589920	1.5879000	0.6484830	C	5.4917090	-0.3423830	-0.7071110
C	3.7921670	1.3011000	1.1513730	C	4.1970810	-0.6845760	-1.0916640
C	-1.1823900	1.5598890	-0.9741790	C	-2.4095240	-0.7458170	-0.8918160
C	-1.4715510	2.8799230	-0.5696330	C	-3.7920560	-0.8467580	-0.6343730
C	-1.4455880	3.9241460	-1.4886360	C	-4.5982390	-1.6776560	-1.4077290
C	-1.1436140	3.6723340	-2.8313610	C	-4.0443580	-2.4186120	-2.4561560
C	-0.8680350	2.3677350	-3.2490970	C	-2.6764640	-2.3226100	-2.7255340
C	-0.8832640	1.3196910	-2.3325990	C	-1.8607700	-1.4949420	-1.9560040
C	-2.2976370	0.4619630	1.0317980	C	-2.0441950	1.4733470	0.3121630
C	-3.6258110	0.7992060	0.7054790	C	-1.6981120	2.0069140	1.5726260
C	-4.6159290	0.8072270	1.6854480	C	-2.1896240	3.2450920	1.9757130
C	-4.2983910	0.4873340	3.0086430	C	-3.0277980	3.9779210	1.1309140
C	-2.9808580	0.1664290	3.3467680	C	-3.3787940	3.4617060	-0.1209630
C	-1.9843530	0.1548970	2.3718700	C	-2.8970520	2.2208540	-0.5267660
H	1.8087420	-1.4221050	1.9070360	H	1.2709800	0.8023010	-2.1672250
H	0.0032170	-2.4567060	0.7798530	H	0.9321920	-1.9300060	0.0809790
H	-1.6656860	-1.9115600	0.9362860	H	-0.7879750	-2.2959890	0.1843850
H	3.8304520	-2.0895590	0.8246300	H	2.8941340	2.4399310	-1.4623880
H	6.0943160	-1.5798200	-0.0671030	H	5.2057030	3.0523930	-0.7881680
H	6.8789700	0.7764440	-0.1819890	H	6.8682530	1.2695170	-0.2976580
H	5.4033100	2.6175360	0.5990510	H	6.2196290	-1.1218060	-0.4975670
H	3.1343890	2.0902600	1.5024130	H	3.8981540	-1.7233890	-1.1949090
H	-1.6969360	3.0808340	0.4728150	H	-4.2249490	-0.2835210	0.1863080
H	-1.6573140	4.9371320	-1.1583260	H	-5.6597490	-1.7513830	-1.1889300
H	-1.1301710	4.4883350	-3.5485200	H	-4.6757530	-3.0635400	-3.0607910
H	-0.6482870	2.1646150	-4.2934540	H	-2.2426340	-2.8862310	-3.5468990
H	-0.7110100	0.3005940	-2.6628170	H	-0.7999860	-1.4101890	-2.1832330
H	-3.8790180	1.0369430	-0.3231490	H	-1.0773730	1.4186170	2.2408230
H	-5.6375930	1.0590140	1.4150420	H	-1.9244650	3.6360470	2.9539100
H	-5.0711600	0.4967540	3.7722200	H	-3.4104400	4.9441590	1.4474970
H	-2.7236150	-0.0599590	4.3779690	H	-4.0252550	4.0305230	-0.7831480
H	-0.9483040	-0.0368680	2.6388910	H	-3.1631950	1.8302490	-1.5036160
C	-1.2121080	-2.7424430	-0.9830440	C	0.0773040	-1.8603110	2.0819910
O	-1.5076030	-2.2626420	-2.0556220	O	-0.4614630	-1.1657580	2.9167620
O	-1.2292710	-4.0489360	-0.6939670	O	0.7830940	-2.9666630	2.3450730
C	-1.6557320	-4.9275950	-1.7588340	C	0.8711490	-3.3449900	3.7363360
H	-0.9826120	-4.8360140	-2.6139190	H	-0.1265080	-3.5216740	4.1444660
H	-1.6111470	-5.9318440	-1.3398110	H	1.4601450	-4.2610080	3.7498550
H	-2.6749100	-4.6823690	-2.0656060	H	1.3679760	-2.5589480	4.3090910
Molecule 17				TS⁶			
E = -1407.24383826, H (0K) = -1406.843406, H (298K) = -1406.816197, G (298K) = -1406.902023 au				E = -1407.23663505, H (0K) = -1406.836629, H (298K) = -1406.809951, G (298K) = -1406.894894 au			

Imaginary frequency = 0.				Imaginary frequency = 1.			
C	1.4325840	-0.2642170	-0.0162700	C	-1.8685140	-0.0437170	0.4730580C
O	-1.3495390	0.9068120	-1.8768360	O	-1.3990860	-0.2263290	-0.0448010
C	-1.5762360	-0.1598390	-1.1223410	O	0.8103730	-0.1797380	1.9313910
C	-0.9987380	0.0028280	0.3785500	C	1.3868570	-0.7591730	0.8891930
N	0.3847160	0.5204360	0.2775450	C	1.0103930	-0.0237830	-0.4969770
C	0.3938220	1.9800130	0.0932210	N	-0.3685590	0.5498740	-0.3775420
F	-1.0391500	-1.1751720	1.0441500	C	-0.3662290	1.9901860	-0.0755090
F	-1.7203450	0.8945820	1.1098220	F	1.1143800	-0.8522570	-1.5673360
C	-3.0562640	-0.5712790	-0.9826190	F	1.8287780	1.0315810	-0.7666880
C	-3.4475740	-1.8728150	-0.6449260	C	2.9329770	-0.8175460	0.9173110
C	-4.8009280	-2.2074450	-0.5521990	C	3.6639520	-1.6848820	0.0962810
C	-5.7793520	-1.2388310	-0.7909610	C	5.0585100	-1.7278540	0.1709010
C	-5.3955400	0.0628010	-1.1291800	C	5.7377270	-0.9001330	1.0693000
C	-4.0427620	0.3901000	-1.2256780	C	5.0124720	-0.0342120	1.8934840
C	2.3935630	0.1489910	-1.0449030	C	3.6192430	0.0025280	1.8167300
C	3.7759470	-0.0730290	-0.8826790	C	-2.4783130	0.2487900	0.8404310
C	4.6599000	0.2735750	-1.8996070	C	-3.8221370	0.1243240	0.4406170
C	4.1742090	0.8169420	-3.0936150	C	-4.8410500	0.5473950	1.2901880
C	2.8015430	1.0215460	-3.2693020	C	-4.5308390	1.0577200	2.5542260
C	1.9071840	0.7030910	-2.2516240	C	-3.1984670	1.1497260	2.9693880
C	1.6466900	-1.5148030	0.7135430	C	-2.1685820	0.7543320	2.1202810
C	1.4308280	-1.5466420	2.1086370	C	-1.5599250	-1.5577090	-0.6451710
C	1.7247100	-2.6968010	2.8327250	C	-1.4026250	-1.7319470	-2.0349470
C	2.2160150	-3.8307520	2.1785020	C	-1.6724580	-2.9684200	-2.6143050
C	2.4321180	-3.8094990	0.7961660	C	-2.0751010	-4.0433330	-1.8175050
C	2.1653320	-2.6557860	0.0672040	C	-2.2350570	-3.8775030	-0.4373100
H	-0.9976650	-1.0825820	-1.4138790	C	-2.0037490	-2.6364680	0.1453460
H	-0.4327120	2.2435170	-0.5748380	H	1.0449010	-1.8069700	0.6667580
H	1.3286600	2.2844260	-0.3765590	H	0.3456540	2.1985690	0.7230510
H	-2.6906290	-2.6319310	-0.4611210	H	-1.3581920	2.2822100	0.2670540
H	-5.0913750	-3.2240080	-0.2978610	H	3.1402100	-2.3341760	-0.6022380
H	-6.8328420	-1.4978930	-0.7207450	H	5.6143570	-2.4101170	-0.4680650
H	-6.1527540	0.8193090	-1.3219900	H	6.8225130	-0.9359770	1.1321560
H	-3.7163320	1.3855440	-1.5110320	H	5.5348130	0.6068320	2.6002410
H	4.1494500	-0.4920840	0.0459070	H	3.0263240	0.6463490	2.4591960
H	5.7260350	0.1194900	-1.7641050	H	-4.0595160	-0.2762740	-0.5397760
H	4.8666550	1.0780310	-3.8888670	H	-5.8757590	0.4719060	0.9701110
H	2.4279160	1.4272730	-4.2048590	H	-5.3289180	1.3726280	3.2205000
H	0.8297300	0.8387760	-2.3765770	H	-2.9624160	1.5199290	3.9626950
H	1.0770720	-0.6507720	2.6081460	H	-1.1248290	0.7605550	2.4232260
H	1.5748910	-2.7091560	3.9079830	H	-1.1064090	-0.8888670	-2.6480690
H	2.4375940	-4.7297180	2.7464570	H	-1.5697930	-3.0924690	-3.6879460
H	2.8100710	-4.6922470	0.2896800	H	-2.2742780	-5.0091910	-2.2726950
H	2.3266070	-2.6383660	-1.0055440	H	-2.5486270	-4.7134160	0.1802270
C	0.3123020	2.6651230	1.4529850	H	-2.1318210	-2.4992330	1.2139280
O	0.6067850	2.1597050	2.5160470	C	-0.0649250	2.7877710	-1.3398170
O	-0.0778020	3.9352630	1.2917330	O	-0.2530440	2.3930520	-2.4703390
C	-0.1225160	4.7405240	2.4896310	O	0.3750320	4.0072440	-1.0113890
H	0.8651110	4.7845260	2.9542590	C	0.6254140	4.9066890	-2.1138550
H	-0.4372480	5.7300310	2.1608190	H	-0.2895660	5.0643270	-2.6891680
H	-0.8423530	4.3230860	3.1970410	H	0.9580180	5.8376140	-1.6568750
				H	1.4019240	4.4972730	-2.7635030
Molecule conformer of 18 (from TS ⁶)				TS ⁷			
E = -1407.31281826, H (0K) = -1406.909916, H (298K) = -1406.883088, G (298K) = -1406.969638 au				E = -1407.23419132, H (0K) = -1406.838344, H (298K) = -1406.811373, G (298K) = -1406.896958 au			
Imaginary frequency = 0.				Imaginary frequency = 1.			
C	-0.4890620	-0.7719670	-0.0561730	C	1.1919540	0.5154000	0.2041270
O	0.9140890	-1.1053190	-0.1437740	O	-1.9649590	-2.3626670	0.2468680
C	1.5965150	0.0173050	-0.6917760	C	-2.1362200	-1.1040210	0.7674760

C	0.8404460	1.1823300	-0.0385300	C	-1.2081140	-0.0881700	0.0166190
N	-0.4757170	0.7139230	0.0650120	N	0.2350940	-0.4053840	0.1857260
C	-1.4177460	1.4499250	0.8851630	C	0.5324190	-1.8591820	0.1544110
F	0.9458700	2.3426020	-0.7646700	F	-1.4222420	1.1733450	0.4775540
F	1.3836080	1.5158010	1.1977090	F	-1.5007510	-0.0987160	-1.3152280
C	3.0778310	-0.0295430	-0.4149820	C	-3.5810840	-0.6126760	0.6601420
C	3.9350520	0.7597120	-1.1919190	C	-4.1196670	0.2897900	1.5844270
C	5.3074850	0.7668810	-0.9413060	C	-5.4445740	0.7168360	1.4717620
C	5.8356830	-0.0248330	0.0815320	C	-6.2446640	0.2454690	0.4279350
C	4.9840510	-0.8184330	0.8531670	C	-5.7125770	-0.6563570	-0.4981470
C	3.6089740	-0.8177830	0.6109930	C	-4.3887290	-1.0821970	-0.3815310
C	-1.0322370	-1.4435310	1.2094570	C	2.5006330	0.1828180	0.7982190
C	-2.2763910	-2.0830250	1.2433370	C	3.6850830	0.5399470	0.1292710
C	-2.7506120	-2.6478020	2.4315200	C	4.9223380	0.2635940	0.7063890
C	-1.9861080	-2.5786310	3.5955240	C	4.9884190	-0.3312820	1.9687300
C	-0.7466630	-1.9310980	3.5715760	C	3.8140110	-0.6594940	2.6540280
C	-0.2757680	-1.3639670	2.3895000	C	2.5750720	-0.4188520	2.0689550
C	-1.1679930	-1.2424290	-1.3498270	C	1.0337280	1.8695330	-0.3458090
C	-1.9123240	-0.3843490	-2.1639670	C	0.5020740	2.0601110	-1.6367100
C	-2.4962820	-0.8628740	-3.3424750	C	0.4519220	3.3392720	-2.1821320
C	-2.3356140	-2.1953200	-3.7200300	C	0.9026070	4.4375390	-1.4444250
C	-1.5836080	-3.0557540	-2.9131380	C	1.4340500	4.2549090	-0.1639660
C	-1.0056020	-2.5825720	-1.7372040	C	1.5241470	2.9759670	0.3753310
H	1.4154060	0.0910830	-1.7740950	H	-1.8286000	-1.0029900	1.8326720
H	-0.9792470	1.7607170	1.8393130	H	-0.6919380	-2.3553800	0.1034250
H	-2.2611520	0.7960660	1.1269710	H	0.9246270	-2.2308420	1.0970480
H	3.5267840	1.3709770	-1.9930140	H	-3.5016480	0.6558660	2.4012040
H	5.9634530	1.3836380	-1.5493870	H	-5.8527900	1.4121680	2.2009100
H	6.9053360	-0.0265990	0.2724930	H	-7.2773070	0.5734350	0.3407390
H	5.3895960	-1.4400000	1.6469040	H	-6.3315430	-1.0304960	-1.3099480
H	2.9472990	-1.4385750	1.2051610	H	-3.9645930	-1.7963830	-1.0791710
H	-2.8777970	-2.1476300	0.3429970	H	3.6298570	1.0038330	-0.8496400
H	-3.7173310	-3.1434770	2.4408530	H	5.8333380	0.5199950	0.1745970
H	-2.3525520	-3.0217380	4.5174220	H	5.9540510	-0.5327160	2.4231980
H	-0.1474310	-1.8667980	4.4756550	H	3.8644380	-1.1022890	3.6439290
H	0.6771760	-0.8459650	2.3757410	H	1.6640400	-0.6583560	2.6079250
H	-2.0224230	0.6591490	-1.8884690	H	0.1748510	1.2031550	-2.2107820
H	-3.0719940	-0.1849330	-3.9671900	H	0.0629170	3.4788340	-3.1860280
H	-2.7875480	-2.5633530	-4.6372570	H	0.8499830	5.4348840	-1.8712860
H	-1.4455250	-4.0941970	-3.2021370	H	1.7878840	5.1072780	0.4076700
H	-0.4171260	-3.2519460	-1.1165550	H	1.9455690	2.8300570	1.3644280
C	-1.9977040	2.6785280	0.1837960	C	1.3770950	-2.1952580	-1.0022860
O	-2.1414490	2.8218240	-1.0121590	O	1.6146250	-1.4797840	-1.9676130
O	-2.3827260	3.5801320	1.1014530	O	1.8330810	-3.4681350	-0.8961180
C	-3.0330430	4.7630810	0.5925650	C	2.5980660	-3.9511290	-2.0118950
H	-3.9361180	4.4928350	0.0402580	H	3.4881270	-3.3354540	-2.1669150
H	-3.2835440	5.3573390	1.4705320	H	2.8836120	-4.9705130	-1.7507630
H	-2.3555340	5.3141450	-0.0636280	H	1.9964990	-3.9487790	-2.9248510
Molecule 19				TS⁸			
E = -1407.24840157, H (0K) = -1406.848334,				E = -1407.24568294, H (0K) = -1406.845590,			
H (298K) = -1406.820778, G (298K) = -1406.907711				H (298K) = -1406.818979, G (298K) = -1406.902338			
au				au			
Imaginary frequency = 0.				Imaginary frequency = 1.			
C	1.1492570	0.5007530	0.1562210	C	1.3997030	0.0610720	0.3753440
O	-2.2097380	-2.2361190	-0.8700080	O	-2.0162130	0.8568010	-1.4340310
C	-2.1702140	-1.3060710	0.1938090	C	-2.1950650	-0.3334820	-0.6962800
C	-1.2183260	-0.1234930	-0.1540500	C	-1.0965130	-0.4789770	0.3854240
N	0.2210870	-0.4570800	-0.0343480	N	0.2229110	-0.4541870	-0.1528730
C	0.6048520	-1.7928850	-0.2355590	C	0.6867580	-1.1188500	-1.2969220
F	-1.4628280	0.9215890	0.6787640	F	-1.3157280	-1.6831280	1.0453610
F	-1.4950600	0.2902310	-1.4226990	F	-1.1855440	0.4870340	1.3375930

C	-3.5760390	-0.7930560	0.4440040	C	-3.5763540	-0.3387630	-0.0695990
C	-4.0262000	-0.5809480	1.7513220	C	-4.2657530	-1.5428970	0.1120560
C	-5.3161900	-0.1017270	1.9857630	C	-5.5286470	-1.5530510	0.7068200
C	-6.1667970	0.1676990	0.9114660	C	-6.1138980	-0.3561240	1.1256050
C	-5.7218020	-0.0439360	-0.3961790	C	-5.4291800	0.8487640	0.9473820
C	-4.4312050	-0.5194000	-0.6306710	C	-4.1651100	0.8580700	0.3562260
C	2.3805330	0.1829410	0.9012740	C	2.4225770	-0.9096450	0.8461520
C	3.6183320	0.6934530	0.4776840	C	3.7967800	-0.7252390	0.6067840
C	4.7716240	0.4685240	1.2312050	C	4.7294740	-1.6434320	1.0848410
C	4.7004660	-0.2546430	2.4213870	C	4.3088560	-2.7589020	1.8139490
C	3.4677800	-0.7590660	2.8577860	C	2.9458280	-2.9543280	2.0542470
C	2.3203190	-0.5531670	2.1024730	C	2.0088850	-2.0437190	1.5718140
C	0.9892150	1.8669000	-0.3723180	C	1.5754730	1.4960800	0.5665650
C	0.6667750	2.0865160	-1.7244960	C	0.7116940	2.4251010	-0.0598070
C	0.5797490	3.3851010	-2.2231450	C	0.8610320	3.7905040	0.1544330
C	0.8009940	4.4780100	-1.3825550	C	1.8649300	4.2680450	1.0010600
C	1.1325520	4.2693530	-0.0395970	C	2.7160200	3.3648120	1.6465850
C	1.2440770	2.9753570	0.4590420	C	2.5789790	1.9991170	1.4332870
H	-1.7877460	-1.7546520	1.1220820	H	-2.0850500	-1.2211870	-1.3368300
H	-1.2803800	-2.4547920	-1.0861130	H	-1.1694230	0.8081100	-1.9379700
H	0.1760410	-2.5609460	0.3937800	H	0.8283190	-2.1947590	-1.2937440
H	-3.3683720	-0.7960660	2.5899290	H	-3.8147980	-2.4760910	-0.2156310
H	-5.6570680	0.0545970	3.0054890	H	-6.0560430	-2.4941630	0.8371130
H	-7.1727860	0.5366350	1.0920480	H	-7.0989470	-0.3616250	1.5844790
H	-6.3806730	0.1616000	-1.2354710	H	-5.8797140	1.7837760	1.2697340
H	-4.0844370	-0.6906360	-1.6438130	H	-3.6338830	1.7924310	0.2106070
H	3.6747210	1.2521950	-0.4500120	H	4.1299760	0.1252730	0.0199060
H	5.7238050	0.8607950	0.8858350	H	5.7854600	-1.4919470	0.8798500
H	5.5963140	-0.4239350	3.0120690	H	5.0371570	-3.4728170	2.1879460
H	3.4045390	-1.3089720	3.7924450	H	2.6107170	-3.8178500	2.6219770
H	1.3673890	-0.9438150	2.4458850	H	0.9509280	-2.2007070	1.7549680
H	0.5248140	1.2373710	-2.3818070	H	-0.0689900	2.0656140	-0.7120170
H	0.3460440	3.5417420	-3.2722060	H	0.1911710	4.4859790	-0.3426250
H	0.7263710	5.4888840	-1.7732100	H	1.9789510	5.3359130	1.1646100
H	1.3097520	5.1164300	0.6166620	H	3.4834620	3.7269860	2.3242240
H	1.5074740	2.8140090	1.4996670	H	3.2259550	1.3136130	1.9660670
C	1.7269070	-2.0826730	-1.0669810	C	0.8996900	-0.3732180	-2.5007290
O	2.3817070	-1.2960670	-1.7561800	O	0.4760860	0.7720350	-2.7380630
O	1.9879460	-3.4320950	-1.0603920	O	1.5768770	-1.0915620	-3.4316050
C	3.0254680	-3.8591580	-1.9482840	C	1.7009470	-0.4843910	-4.7267710
H	3.9665310	-3.3460030	-1.7302240	H	2.2984740	0.4295220	-4.6711420
H	3.1339110	-4.9318600	-1.7798540	H	2.2032200	-1.2254050	-5.3493140
H	2.7550550	-3.6714570	-2.9922960	H	0.7174770	-0.2439880	-5.1398960
Molecule 20				Molecule conformer of 18 (from TS⁴)			
E = -1407.28460921, H (0K) = -1406.883303, H (298K) = -1406.855866, G (298K) = -1406.943815 au				E = -1407.30784269, H (0K) = -1406.905033, H (298K) = -1406.878204, G (298K) = -1406.965219 au			
Imaginary frequency = 0.				Imaginary frequency = 0.			
C	1.3300370	0.3262830	0.0496440	C	-0.4831350	-0.7616570	0.0604040
O	-1.9312520	-2.2204030	-0.3310500	O	0.8818520	-1.2028830	-0.0846040
C	-2.2560700	-1.0227690	0.3439530	C	1.6206810	-0.3610330	-0.9691450
C	-1.2587040	0.1048500	-0.0417050	C	0.8210850	0.9548450	-0.9693850
N	0.0625250	-0.4034310	-0.0253480	N	-0.4489110	0.6160750	-0.4866010
C	0.8190680	-0.5492130	1.1892060	C	-1.6152430	1.3402430	-0.9400410
F	-1.4648000	1.1657320	0.8241080	F	0.7701650	1.4918880	-2.2387140
F	-1.4994830	0.5885090	-1.2957950	F	1.4322900	1.9442250	-0.2225880
C	-3.6834810	-0.6240510	0.0299950	C	3.0625620	-0.2612880	-0.5361520
C	-4.4336260	0.0978910	0.9652230	C	4.0747000	-0.2537760	-1.5013830
C	-5.7404760	0.4916210	0.6718930	C	5.4134530	-0.1335640	-1.1215470
C	-6.3093620	0.1640390	-0.5608220	C	5.7480110	-0.0305410	0.2295890
C	-5.5637860	-0.5558980	-1.4980050	C	4.7395400	-0.0449240	1.1982530

C	-4.2553150	-0.9440900	-1.2070230	C	3.4027770	-0.1559810	0.8184850
C	1.3613950	1.8204210	0.2784540	C	-0.7668510	-0.8081550	1.5681910
C	1.8450070	2.3634310	1.4743280	C	-0.9810190	-2.0481540	2.1889950
C	1.9176810	3.7486840	1.6442190	C	-1.1470670	-2.1299560	3.5709540
C	1.5071560	4.6019230	0.6195540	C	-1.1060780	-0.9714800	4.3519790
C	1.0278240	4.0652240	-0.5792130	C	-0.8878650	0.2633580	3.7403280
C	0.9620950	2.6837390	-0.7521650	C	-0.7120740	0.3465650	2.3557830
C	2.4016480	-0.2061050	-0.8797120	C	-1.4278110	-1.6706440	-0.7449560
C	2.0906270	-1.1113290	-1.9015480	C	-2.8002780	-1.7187490	-0.4566970
C	3.0932810	-1.5957690	-2.7443810	C	-3.6659340	-2.4969830	-1.2278260
C	4.4168180	-1.1877500	-2.5713780	C	-3.1696160	-3.2527680	-2.2910950
C	4.7335200	-0.2863930	-1.5514080	C	-1.8021220	-3.2281900	-2.5724020
C	3.7325000	0.2053610	-0.7142160	C	-0.9388430	-2.4438790	-1.8055610
H	-2.1477550	-1.1399870	1.4334550	H	1.5702900	-0.7432780	-1.9977830
H	-1.0005980	-2.4319370	-0.1151590	H	-1.5944720	1.4914420	-2.0252250
H	0.4915060	-0.0091030	2.0767270	H	-2.5093770	0.7470070	-0.7380160
H	-3.9953340	0.3507970	1.9272490	H	3.8166710	-0.3446880	-2.5538750
H	-6.3144460	1.0477960	1.4081320	H	6.1916080	-0.1294860	-1.8797910
H	-7.3285520	0.4646030	-0.7885100	H	6.7891690	0.0557470	0.5284120
H	-6.0012890	-0.8148890	-2.4585640	H	4.9957750	0.0315360	2.2514700
H	-3.6741080	-1.5063480	-1.9298980	H	2.6186770	-0.1719830	1.5686140
H	2.1713900	1.7045420	2.2743630	H	-1.0145490	-2.9533740	1.5901990
H	2.2952690	4.1569340	2.5775810	H	-1.3099280	-3.0979530	4.0371930
H	1.5604130	5.6789620	0.7519110	H	-1.2421120	-1.0334930	5.4283860
H	0.7052370	4.7237820	-1.3808590	H	-0.8519640	1.1695760	4.3393260
H	0.5852710	2.2700460	-1.6828520	H	-0.5347990	1.3071070	1.8849820
H	1.0620810	-1.4303490	-2.0285280	H	-3.1960750	-1.1627750	0.3884640
H	2.8363280	-2.2921820	-3.5379960	H	-4.7254170	-2.5185320	-0.9881940
H	5.1961840	-1.5661680	-3.2271270	H	-3.8405350	-3.8639080	-2.8883410
H	5.7606320	0.0384610	-1.4091520	H	-1.4020690	-3.8257130	-3.3870110
H	3.9848700	0.9156950	0.0678160	H	0.1234750	-2.4533310	-2.0204520
C	1.3167790	-1.9457710	1.4497530	C	-1.8173330	2.7074350	-0.2855830
O	0.8588710	-2.9405400	0.9163450	O	-1.1913270	3.1721850	0.6423950
O	2.2982560	-1.9491880	2.3535540	O	-2.8298810	3.3395140	-0.9044190
C	2.8340960	-3.2441080	2.7092770	C	-3.1710130	4.6433750	-0.3909540
H	3.2704730	-3.7234520	1.8305270	H	-2.3170040	5.3193840	-0.4748870
H	3.5986380	-3.0440320	3.4584360	H	-3.9975140	4.9921550	-1.0091190
H	2.0453990	-3.8776230	3.1207320	H	-3.4778930	4.5718820	0.6551970
Molecule 21				TS⁹			
E = -635.31460004, H (0K) = -635.055443, H (298K) = -635.040588, G (298K) = -635.096783 au Imaginary frequency = 0.				E = -1179.35084247, H (0K) = -1178.997787, H (298K) = -1178.975725, G (298K) = -1179.049784 au Imaginary frequency = 1.			
C	0.0052580	0.6875490	0.0228420	C	-1.4339680	-0.0536740	0.4081140
C	0.9224790	2.8452100	-0.5689350	O	1.4168590	-2.1905820	-0.3704450
N	-0.0292980	2.0603900	-0.0604290	C	1.6497740	-0.8312210	-0.4320200
C	-1.1771670	2.8019370	0.5312650	C	1.0148400	-0.0359030	0.7851800
C	1.3043570	-0.0099780	-0.0542690	N	-0.3641180	-0.5526020	1.0422640
C	1.4474120	-1.1929590	-0.8083820	C	-0.2245040	-1.8794100	1.5530620
C	2.6460970	-1.9088220	-0.8212090	F	1.0259120	1.2788690	0.4835050
C	3.7453120	-1.4611290	-0.0881770	F	1.7351680	-0.1730730	1.9272050
C	3.6261660	-0.2853410	0.6644540	C	3.1367940	-0.4829000	-0.4983340
C	2.4317770	0.4260800	0.6804270	C	3.5736750	0.6795950	-1.1436890
C	-1.2448380	-0.0787030	0.0406450	C	4.9341530	0.9912070	-1.1969260
C	-1.3492130	-1.2661260	0.8049230	C	5.8700080	0.1421640	-0.6020670
C	-2.5238080	-2.0106170	0.8335460	C	5.4381830	-1.0209090	0.0421910
C	-3.6473590	-1.5980580	0.1067170	C	4.0789480	-1.3313040	0.0929620
C	-3.5655930	-0.4358020	-0.6625090	C	-2.5564250	-0.9501300	0.0506690
C	-2.3828960	0.3025490	-0.7078280	C	-3.8831860	-0.5750570	0.3280970
H	-0.7666280	3.5794420	1.1785930	C	-4.9452990	-1.3862890	-0.0683120
H	-1.7919800	2.1271830	1.1193950	C	-4.7001370	-2.5696710	-0.7685790

H	-1.7716240	3.2682440	-0.2559770	C	-3.3854880	-2.9432220	-1.0657020
H	0.6028000	-1.5545490	-1.3874120	C	-2.3200280	-2.1480920	-0.6525190
H	2.7200410	-2.8159740	-1.4161500	C	-1.6005680	1.3882790	0.1299350
H	4.6806710	-2.0138430	-0.1011100	C	-1.3805800	2.3498160	1.1355370
H	4.4692900	0.0723320	1.2506640	C	-1.6388090	3.6969450	0.8946410
H	2.3625230	1.3348070	1.2723890	C	-2.1187120	4.1091670	-0.3515750
H	-0.4933330	-1.5931650	1.3881770	C	-2.3506460	3.1633390	-1.3540830
H	-2.5693200	-2.9132310	1.4382140	C	-2.1062810	1.8132700	-1.1128390
H	-4.5655630	-2.1782010	0.1345290	H	1.1386250	-0.3679110	-1.2970740
H	-4.4202940	-0.1104410	-1.2508630	H	0.6727370	-2.3355120	0.5066370
H	-2.3291800	1.1749360	-1.3529330	H	-1.1815110	-2.3754140	1.6738730
H	0.8802890	3.9057210	-0.3690630	H	0.3805350	-1.8635720	2.4563630
H	1.7694900	2.3992730	-1.0665030	H	2.8491030	1.3414860	-1.6117250
				H	5.2619100	1.8933510	-1.7068370
				H	6.9292940	0.3812290	-0.6458500
				H	6.1622080	-1.6885510	0.5023070
				H	3.7326420	-2.2406810	0.5729620
				H	-4.0767400	0.3498200	0.8624650
				H	-5.9641360	-1.0914080	0.1659320
				H	-5.5285510	-3.1975970	-1.0840870
				H	-3.1901430	-3.8557950	-1.6215140
				H	-1.2995270	-2.4395250	-0.8843440
				H	-1.0249100	2.0314580	2.1105740
				H	-1.4717690	4.4250640	1.6832700
				H	-2.3188600	5.1605820	-0.5374660
				H	-2.7247260	3.4770270	-2.3244440
				H	-2.2924050	1.0806670	-1.8921710
TS¹⁰				Molecule 22			
E = -980.89552844, H (0K) = -980.524247,				E = -980.95066503, H (0K) = -980.574242,			
H (298K) = -980.502442, G (298K) = -980.576489 au				H (298K) = -980.553736, G (298K) = -980.623599 au			
Imaginary frequency = 1.				Imaginary frequency = 0.			
O	-0.5618450	-1.4020320	-1.0840910	C	0.7894640	-0.2037120	0.3318700
C	-1.4933230	-1.7287710	-0.3208070	O	-0.3018580	-0.7793810	-0.4539300
C	-0.8459240	-0.7341400	1.6679290	C	-1.3305480	-1.2553330	0.4290400
N	0.4946480	-0.8604150	1.4312540	C	-0.9181140	-0.6495240	1.7911670
C	1.0813380	-2.1224610	1.9357680	N	0.5476620	-0.6066410	1.7255970
C	-2.8498070	-1.1063830	-0.3800610	C	1.1603520	-1.8696210	2.1639750
C	-3.9236820	-1.6786480	0.3176540	C	-2.7144870	-0.8755350	-0.0447030
C	-5.1998390	-1.1217990	0.2361590	C	-3.7645690	-1.7929690	0.0886420
C	-5.4177810	0.0151610	-0.5481790	C	-5.0658140	-1.4494810	-0.2843840
C	-4.3525110	0.5877770	-1.2519270	C	-5.3309600	-0.1823780	-0.8072910
C	-3.0780480	0.0294210	-1.1715390	C	-4.2873950	0.7362890	-0.9521550
C	0.7720830	1.3447730	0.3910700	C	-2.9890870	0.3940200	-0.5723310
C	0.7894750	1.8814730	-0.9081280	C	0.7128200	1.3286720	0.1895660
C	0.4641140	3.2190230	-1.1337470	C	0.4851870	1.8910870	-1.0753090
C	0.1205330	4.0502510	-0.0652270	C	0.4533720	3.2753030	-1.2420000
C	0.1076460	3.5319700	1.2335350	C	0.6516900	4.1207610	-0.1457310
C	0.4298350	2.1955450	1.4602710	C	0.8827050	3.5685410	1.1143010
C	2.5029020	-0.4817730	0.0482270	C	0.9166080	2.1802690	1.2802410
C	3.6415100	0.3337230	0.2036520	C	2.1208650	-0.7106660	-0.2314880
C	4.8687600	-0.0423290	-0.3387810	C	3.3288500	-0.1402550	0.1969150
C	4.9838580	-1.2352750	-1.0587130	C	4.5481180	-0.6088990	-0.2913530
C	3.8577580	-2.0420280	-1.2403190	C	4.5781590	-1.6460920	-1.2280590
C	2.6275260	-1.6686420	-0.6998940	C	3.3799130	-2.2103220	-1.6663730
H	-1.4786120	-2.7109100	0.1918100	C	2.1580950	-1.7480190	-1.1691660
H	0.6693950	-2.3092010	2.9282580	H	-1.2656150	-2.3514370	0.4791460
H	2.1629280	-2.0314250	2.0011260	H	0.8527800	-2.0472420	3.1986220
H	0.8190730	-2.9501810	1.2738340	H	2.2476850	-1.7819900	2.1451560
H	-3.7532360	-2.5657010	0.9251570	H	0.8771540	-2.7477780	1.5625560
H	-6.0249540	-1.5744220	0.7801320	H	-3.5614800	-2.7853190	0.4857160
H	-6.4115560	0.4501530	-0.6134650	H	-5.8681970	-2.1741990	-0.1741320

H	-4.5199280	1.4687470	-1.8665930	H	-6.3410190	0.0860160	-1.1050960
H	-2.2424850	0.4588320	-1.7162290	H	-4.4848710	1.7224080	-1.3646420
H	1.0484890	1.2350900	-1.7406880	H	-2.1805500	1.1078390	-0.6954940
H	0.4761000	3.6108620	-2.1473500	H	0.3273830	1.2377450	-1.9279950
H	-0.1322040	5.0922840	-0.2405980	H	0.2737730	3.6950270	-2.2283980
H	-0.1452700	4.1730690	2.0738850	H	0.6264400	5.1994100	-0.2754820
H	0.4247540	1.8058800	2.4746070	H	1.0370260	4.2159220	1.9737750
H	3.5599140	1.2610390	0.7634660	H	1.0913510	1.7456890	2.2589910
H	5.7373640	0.5953280	-0.1973740	H	3.3151810	0.6760850	0.9132090
H	5.9404600	-1.5269330	-1.4836740	H	5.4747230	-0.1586500	0.0546450
H	3.9325380	-2.9581800	-1.8204470	H	5.5276500	-2.0060290	-1.6150580
H	1.7367980	-2.2580650	-0.8882920	H	3.3910210	-3.0133270	-2.3987940
H	-1.2306620	-1.2784760	2.5216320	H	1.2269070	-2.1835480	-1.5118820
H	-1.2973750	0.2160420	1.4302680	H	-1.2607460	-1.2348980	2.6469620
				H	-1.3167080	0.3669950	1.8782070
TS11				Molecule 23			
E = -980.89381064, H (0K) = -980.521684, H (298K) = -980.500322, G (298K) = -980.572869 au Imaginary frequency = 1.				E = -980.89976328, H (0K) = -980.525301, H (298K) = -980.504207, G (298K) = -980.575609 au Imaginary frequency = 0.			
C	-1.3346680	0.0339230	0.5316470	C	-1.3279520	0.0078930	0.5553050
O	1.4610080	-2.0541250	-0.6786160	O	1.3544890	-2.2258440	-0.3870720
C	1.8320520	-0.8501860	-0.6820150	C	1.6292310	-0.9347330	-0.3138920
C	1.0375040	0.1950290	1.0097950	C	1.0625630	-0.1843510	1.0438450
N	-0.2093800	-0.4005040	1.1174760	N	-0.3288760	-0.5836090	1.1897420
C	-0.1451970	-1.7096080	1.8047830	C	-0.4243130	-1.9117500	1.8163140
C	3.2702660	-0.4760710	-0.4614410	C	3.1263640	-0.5630590	-0.3388520
C	3.7385970	0.8065800	-0.7811810	C	3.5693940	0.7236910	-0.6721810
C	5.0802240	1.1397670	-0.5927630	C	4.9322710	1.0307800	-0.6826710
C	5.9715890	0.1912400	-0.0817740	C	5.8728550	0.0494040	-0.3562220
C	5.5132110	-1.0924920	0.2327980	C	5.4396770	-1.2388980	-0.0278600
C	4.1726960	-1.4242370	0.0408000	C	4.0764530	-1.5396790	-0.0230350
C	-2.4055240	-0.9118890	0.1610380	C	-2.5108410	-0.7666800	0.1290670
C	-3.7555510	-0.6011640	0.4173460	C	-3.8137220	-0.2776280	0.3292880
C	-4.7696810	-1.4784910	0.0408320	C	-4.9104630	-1.0031610	-0.1303480
C	-4.4584740	-2.6763110	-0.6104300	C	-4.7177390	-2.2048030	-0.8187760
C	-3.1247530	-2.9876630	-0.8872370	C	-3.4239970	-2.6838650	-1.0447960
C	-2.1044170	-2.1149420	-0.5114030	C	-2.3220070	-1.9756450	-0.5708390
C	-1.5016210	1.4679640	0.2019470	C	-1.2812370	1.4544180	0.2429280
C	-1.1973970	2.4732310	1.1428600	C	-0.8929700	2.3863030	1.2249770
C	-1.4251040	3.8146300	0.8504610	C	-0.9165770	3.7508290	0.9496960
C	-1.9585210	4.1865220	-0.3886990	C	-1.3200960	4.2069370	-0.3090980
C	-2.2703850	3.2017800	-1.3274780	C	-1.7149250	3.2911560	-1.2871160
C	-2.0499610	1.8557290	-1.0341450	C	-1.7084410	1.9249800	-1.0113440
H	1.2819490	-0.1200900	-1.3125310	H	1.1193170	-0.3056740	-1.0963570
H	0.4558040	-2.3876380	1.1933710	H	0.2109730	-2.5735560	1.2066390
H	-1.1446880	-2.1053490	1.9634550	H	-1.4559020	-2.2510920	1.8633180
H	0.3439120	-1.5448850	2.7677180	H	-0.0133310	-1.8213550	2.8258960
H	3.0468330	1.5433080	-1.1859220	H	2.8426370	1.4900780	-0.9396790
H	5.4325530	2.1359670	-0.8479960	H	5.2610090	2.0323490	-0.9503510
H	7.0172410	0.4488140	0.0645880	H	6.9341710	0.2849000	-0.3660890
H	6.2051180	-1.8352890	0.6222400	H	6.1670850	-2.0096080	0.2176090
H	3.8022060	-2.4200950	0.2651170	H	3.7128030	-2.5371210	0.2054400
H	-4.0025970	0.3270190	0.9242140	H	-3.9619350	0.6601500	0.8559350
H	-5.8047620	-1.2288750	0.2574370	H	-5.9152520	-0.6292450	0.0430690
H	-5.2512870	-3.3572940	-0.9073430	H	-5.5747580	-2.7627050	-1.1853560
H	-2.8774950	-3.9074250	-1.4104660	H	-3.2728690	-3.6074250	-1.5959900
H	-1.0682440	-2.3381270	-0.7543360	H	-1.3079080	-2.3246780	-0.7553340
H	-0.7916000	2.1947230	2.1112890	H	-0.5946500	2.0370740	2.2091620
H	-1.1943160	4.5726670	1.5939240	H	-0.6265980	4.4594510	1.7199460
H	-2.1328680	5.2344690	-0.6157100	H	-1.3330770	5.2717450	-0.5230320
H	-2.6855710	3.4793390	-2.2924110	H	-2.0310930	3.6399500	-2.2657960

H	-2.2966360	1.0953320	-1.7687480	H	-2.0175090	1.2158910	-1.7726110
H	1.0464750	1.2144530	0.6492080	H	1.1635240	0.8903580	0.9250020
H	1.7062760	-0.0245280	1.8350580	H	1.6184110	-0.5202970	1.9206170
TS12				Molecule 24			
E = -980.89371573, H (0K) = -980.519846, H (298K) = -980.499166, G (298K) = -980.570250 au Imaginary frequency = 1.				E = -1179.35507325, H (0K) = -1178.998883, H (298K) = -1178.975590, G (298K) = -1179.052749 au Imaginary frequency = 0.			
C	-1.2373090	-0.0102110	0.5262070	C	-1.4172690	-0.0242910	0.3159620
O	1.0831330	-0.9696230	-1.1282650	O	1.6665040	-2.3949670	0.1592840
C	1.6972260	0.0573020	-0.5836080	C	1.6529150	-1.0288850	-0.2073710
C	1.0939930	0.4795030	0.9632740	C	1.0077970	-0.1481490	0.9016670
N	-0.1161010	-0.2905770	1.1565310	C	1.0077970	-0.1481490	0.9016670
C	0.1712550	-1.6422960	1.6603000	N	-0.4258290	-0.5265020	1.1429930
C	3.2148070	-0.0827380	-0.3670390	C	-0.5870030	-1.5453760	2.0017450
C	4.0164970	1.0164070	-0.0275950	F	1.0950890	1.1405920	0.5156280
C	5.3917890	0.8681280	0.1643040	F	1.6764190	-0.2720480	2.0730410
C	5.9884650	-0.3877980	0.0138110	C	3.0765180	-0.5825790	-0.4755580
C	5.1988240	-1.4868350	-0.3359680	C	3.3430150	0.3265040	-1.5050110
C	3.8238970	-1.3312270	-0.5273620	C	4.6496370	0.7533330	-1.7486490
C	-2.2627250	-1.0424520	0.2434800	C	5.6996340	0.2720180	-0.9640740
C	-3.5828830	-0.8686880	0.6931570	C	5.4374340	-0.6359330	0.0653980
C	-4.5531720	-1.8233100	0.3947790	C	4.1314300	-1.0594200	0.3126470
C	-4.2239720	-2.9372730	-0.3831310	C	-2.5253150	-0.9256920	-0.0753420
C	-2.9206660	-3.0962050	-0.8613480	C	-3.8699340	-0.5234180	0.0394800
C	-1.9379710	-2.1572120	-0.5509310	C	-4.9131760	-1.3402030	-0.4041670
C	-1.5556500	1.3834200	0.1292290	C	-4.6444430	-2.5874640	-0.9662020
C	-1.4934990	2.4321900	1.0641080	C	-3.3128940	-3.0077480	-1.0876180
C	-1.8618750	3.7238410	0.6938060	C	-2.2761040	-2.1915700	-0.6527320
C	-2.2832090	3.9861270	-0.6129150	C	-1.5646740	1.4264790	0.1329770
C	-2.3507310	2.9480510	-1.5452930	C	-1.2946690	2.3454470	1.1710480
C	-2.0043250	1.6497960	-1.1743720	C	-1.4798860	3.7146860	0.9898140
H	1.5419080	1.0316500	-1.1178910	C	-1.9617410	4.2095350	-0.2248440
H	0.7430230	-2.1499940	0.8769260	C	-2.2549790	3.3132950	-1.2583500
H	-0.7494200	-2.1777280	1.8812910	C	-2.0587210	1.9460780	-1.0839210
H	0.7713460	-1.5422900	2.5668840	H	1.0357610	-0.8558160	-1.0993930
H	3.5622100	2.0011860	0.0778690	H	0.7511480	-2.7019990	0.2726390
H	5.9996630	1.7316530	0.4249830	H	-1.5917360	-1.8809000	2.2062500
H	7.0595800	-0.5052560	0.1584780	H	0.2748640	-2.0545070	2.3998460
H	5.6580110	-2.4644620	-0.4667980	H	2.5282100	0.6991620	-2.1203610
H	3.1906710	-2.1633330	-0.8211380	H	4.8459510	1.4561640	-2.5535080
H	-3.8410040	0.0036390	1.2863490	H	6.7177060	0.5999740	-1.1554080
H	-5.5672100	-1.6938660	0.7616840	H	6.2510750	-1.0147070	0.6779020
H	-4.9852670	-3.6736080	-0.6251630	H	3.9270570	-1.7677060	1.1083490
H	-2.6694230	-3.9496230	-1.4847590	H	-4.0962980	0.4429150	0.4796990
H	-0.9259600	-2.2360990	-0.9364850	H	-5.9400480	-0.9989700	-0.2994830
H	-1.1754910	2.2280650	2.0824300	H	-5.4545210	-3.2251150	-1.3087910
H	-1.8235080	4.5246600	1.4264710	H	-3.0844300	-3.9706340	-1.5373830
H	-2.5641400	4.9951270	-0.9008300	H	-1.2506380	-2.5331000	-0.7742980
H	-2.6788060	3.1471130	-2.5612440	H	-0.9474440	1.9749060	2.1316510
H	-2.0609170	0.8411670	-1.8960960	H	-1.2623510	4.3968700	1.8079870
H	0.8967800	1.5468910	0.9771590	H	-2.1131130	5.2765590	-0.3629210
H	1.7929930	0.2250230	1.7589230	H	-2.6296920	3.6833360	-2.2094830
				H	-2.2817290	1.2620330	-1.8979310
TS1'				Molecule 13'			
E = -1179.34788299, H (0K) = -1178.992091, H (298K) = -1178.969137, G (298K) = -1179.043830 au Imaginary frequency = 1.				E = -1179.44326484, H (0K) = -1179.082557, H (298K) = -1179.060625, G (298K) = -1179.132622 au Imaginary frequency = 0.			
C	1.0553330	0.0698160	0.5458950	C	0.5209640	-0.0391690	0.0972390
O	-0.3903170	2.3761980	-0.9207810	O	0.1526110	2.1992210	-0.6087250

C	-0.5530470	1.2351840	-1.4407040	C	-0.2782570	0.8531770	-0.9349830
C	-0.0092990	2.1482220	1.0963870	C	0.6713950	2.2311000	0.6539180
N	1.0911550	1.3995820	1.0207460	N	0.6023830	0.9403830	1.2097680
C	2.3565220	2.1565600	1.2127400	C	1.4551080	0.6900270	2.3696210
F	-1.1722360	1.6006600	1.3669470	F	-0.0045130	3.1471570	1.4281790
F	0.0854060	3.3614170	1.6046350	F	1.9473520	2.7565480	0.6008290
C	-1.8491960	0.5573560	-1.5389060	C	-1.7919100	0.7685550	-0.9347720
C	-1.9348500	-0.6737360	-2.2150020	C	-2.4255480	-0.0498070	-1.8781740
C	-3.1617490	-1.3169980	-2.3672160	C	-3.8170480	-0.1497410	-1.9157630
C	-4.3226180	-0.7380080	-1.8473000	C	-4.5937960	0.5816190	-1.0151500
C	-4.2499720	0.4904600	-1.1780210	C	-3.9694980	1.4125230	-0.0818100
C	-3.0270150	1.1347280	-1.0258150	C	-2.5776670	1.5073680	-0.0407060
C	2.1707430	-0.3648060	-0.3097510	C	1.9381920	-0.3964980	-0.4204110
C	2.7387570	-1.6537900	-0.1844050	C	2.6572220	-1.4456900	0.1758360
C	3.7900340	-2.0677380	-0.9992600	C	3.9652090	-1.7404210	-0.2117570
C	4.3296540	-1.2079950	-1.9600920	C	4.5885480	-0.9893370	-1.2090370
C	3.7934060	0.0754830	-2.0946470	C	3.8939440	0.0656850	-1.8013380
C	2.7311740	0.4868620	-1.2933810	C	2.5880470	0.3633480	-1.4063920
C	0.2014450	-0.8870140	1.2622640	C	-0.2814480	-1.2844920	0.4883720
C	-0.1600960	-0.7044080	2.6164140	C	-1.1050550	-1.2987450	1.6204230
C	-0.9629080	-1.6267130	3.2844770	C	-1.8741710	-2.4227890	1.9305330
C	-1.4257410	-2.7709450	2.6305590	C	-1.8443880	-3.5469300	1.1047720
C	-1.0728360	-2.9758180	1.2928750	C	-1.0398550	-3.5369490	-0.0368080
C	-0.2809760	-2.0503690	0.6190920	C	-0.2640000	-2.4177180	-0.3392380
H	0.2697230	0.7757170	-2.0020420	H	0.0791530	0.6432330	-1.9440320
H	2.4632620	2.9475400	0.4682950	H	2.5223230	0.6594610	2.1198610
H	3.1833020	1.4580170	1.1315870	H	1.1690180	-0.2600550	2.8249220
H	2.3434470	2.5961540	2.2118650	H	1.2807540	1.4847520	3.0995560
H	-1.0322090	-1.1170160	-2.6293130	H	-1.8272250	-0.6124400	-2.5906810
H	-3.2141510	-2.2669730	-2.8921060	H	-4.2921710	-0.7893460	-2.6545480
H	-5.2804130	-1.2372380	-1.9657130	H	-5.6777250	0.5121370	-1.0463470
H	-5.1536110	0.9448730	-0.7804170	H	-4.5671320	1.9939710	0.6151300
H	-2.9640730	2.0908040	-0.5169670	H	-2.1039310	2.1680580	0.6765900
H	2.3556400	-2.3319040	0.5705700	H	2.1881530	-2.0495430	0.9457710
H	4.2009460	-3.0660130	-0.8702160	H	4.4930840	-2.5610940	0.2664880
H	5.1520880	-1.5316540	-2.5917140	H	5.6041860	-1.2206830	-1.5179390
H	4.1940440	0.7589200	-2.8391260	H	4.3671040	0.6665600	-2.5732160
H	2.3165260	1.4803180	-1.4365690	H	2.0927880	1.2112800	-1.8660700
H	0.2159120	0.1586070	3.1583630	H	-1.1552510	-0.4201150	2.2535480
H	-1.2161100	-1.4551530	4.3278580	H	-2.5004430	-2.4140240	2.8185980
H	-2.0478010	-3.4918980	3.1536220	H	-2.4432050	-4.4209930	1.3456450
H	-1.4282920	-3.8572850	0.7649980	H	-1.0114750	-4.4023030	-0.6934440
H	-0.0329060	-2.2191760	-0.4234080	H	0.3629380	-2.4293480	-1.2257330
TS2'							
E = -1179.34640199, H (0K) = -1178.990849,							
H (298K) = -1178.967795, G (298K) = -1179.042788							
au							
Imaginary frequency = 1.							
C	-0.8901200	0.1810250	0.6535420				
O	0.2391200	-2.5951700	-0.4753160				
C	0.5068260	-1.6140060	-1.2128350				
C	-1.5151150	-2.1439460	0.5936360				
N	-1.1495410	-1.0653780	1.2758340				
C	-0.8830290	-1.3161060	2.7193790				
F	-1.8200120	-3.2430870	1.2538280				
F	-2.2033210	-2.0442900	-0.5207900				
C	1.8429330	-1.0359720	-1.3411430				
C	2.0605970	0.0104250	-2.2568680				
C	3.3340230	0.5468320	-2.4263860				
C	4.4102170	0.0388150	-1.6906690				
C	4.2060720	-1.0079910	-0.7844350				

C	2.9331760	-1.5424850	-0.6083490
C	-1.9346930	0.7418030	-0.2143900
C	-3.3083930	0.4766760	-0.0136030
C	-4.2839450	1.0228630	-0.8455720
C	-3.9276610	1.8643040	-1.9021930
C	-2.5742450	2.1477380	-2.1145420
C	-1.5970670	1.5933500	-1.2926130
C	0.1987560	0.9955770	1.1933250
C	1.3804600	0.4213590	1.7241680
C	2.3985910	1.2057050	2.2606220
C	2.2951170	2.5985650	2.2723480
C	1.1436530	3.1907880	1.7428900
C	0.1150970	2.4105230	1.2237280
H	-0.2544150	-1.2293780	-1.9082800
H	-1.8006940	-1.6898230	3.1779700
H	-0.6007960	-0.3735690	3.1769110
H	-0.0845400	-2.0477520	2.8535610
H	1.2237800	0.3955370	-2.8349220
H	3.4915790	1.3570850	-3.1327540
H	5.4051740	0.4535370	-1.8267870
H	5.0437840	-1.4071730	-0.2190160
H	2.7645620	-2.3643170	0.0805730
H	-3.6147870	-0.1500370	0.8195350
H	-5.3311210	0.7986730	-0.6571180
H	-4.6892490	2.2930900	-2.5474920
H	-2.2760850	2.7953990	-2.9354600
H	-0.5504300	1.8118100	-1.4825940
H	1.5086560	-0.6549330	1.6945670
H	3.2886960	0.7216290	2.6553300
H	3.0936130	3.2099170	2.6833450
H	1.0362350	4.2729470	1.7501700
H	-0.7776380	2.8977030	0.8465750