

**A special edition of Organic and Biomolecular Chemistry (OBC)
commemorating the contributions of Athel Beckwith to free radical
chemistry.**

Structural Effects on the Photodissociation of Alkoxyamines

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j.lalevee@uha.fr

i/ Optimized Geometry for **4-6**.

ii/ NMR spectra for the new compounds.

Alkoxyamine 4

C						
C	1	B1				
C	1	B2	2	A1		
H	1	B3	3	A2	2	D1
C	2	B4	1	A3	3	D2
C	3	B5	1	A4	2	D3
C	2	B6	1	A5	3	D4
H	3	B7	1	A6	2	D5
C	5	B8	2	A7	1	D6
C	6	B9	3	A8	1	D7
O	7	B10	2	A9	1	D8
O	7	B11	2	A10	1	D9
H	5	B12	2	A11	1	D10
O	10	B13	6	A12	3	D11
C	10	B14	6	A13	3	D12
C	12	B15	7	A14	2	D13
H	9	B16	5	A15	2	D14
C	15	B17	10	A16	6	D15
C	15	B18	10	A17	6	D16
C	16	B19	12	A18	7	D17
C	16	B20	12	A19	7	D18
H	16	B21	12	A20	7	D19
C	18	B22	15	A21	10	D20
C	19	B23	15	A22	10	D21
C	20	B24	16	A23	12	D22
C	21	B25	16	A24	12	D23
H	18	B26	15	A25	10	D24
H	19	B27	15	A26	10	D25
H	20	B28	16	A27	12	D26
H	20	B29	16	A28	12	D27
H	21	B30	16	A29	12	D28
H	21	B31	16	A30	12	D29
C	24	B32	19	A31	15	D30
N	25	B33	20	A32	16	D31
C	26	B34	21	A33	16	D32
C	26	B35	21	A34	16	D33
C	25	B36	20	A35	16	D34
C	25	B37	20	A36	16	D35
H	23	B38	18	A37	15	D36
H	24	B39	19	A38	15	D37
O	34	B40	25	A39	20	D38
H	33	B41	24	A40	19	D39
H	35	B42	26	A41	21	D40
H	35	B43	26	A42	21	D41
H	35	B44	26	A43	21	D42
H	36	B45	26	A44	21	D43
H	36	B46	26	A45	21	D44
H	36	B47	26	A46	21	D45
H	37	B48	25	A47	20	D46
H	37	B49	25	A48	20	D47

H	37	B50	25	A49	20	D48
H	38	B51	25	A50	20	D49
H	38	B52	25	A51	20	D50
H	38	B53	25	A52	20	D51
C	41	B54	34	A53	25	D52
C	55	B55	41	A54	34	D53
C	55	B56	41	A55	34	D54
H	55	B57	41	A56	34	D55
C	57	B58	55	A57	41	D56
C	57	B59	55	A58	41	D57
H	56	B60	55	A59	41	D58
H	56	B61	55	A60	41	D59
H	56	B62	55	A61	41	D60
C	59	B63	57	A62	55	D61
C	60	B64	57	A63	55	D62
H	59	B65	57	A64	55	D63
H	60	B66	57	A65	55	D64
C	64	B67	59	A66	57	D65
H	64	B68	59	A67	57	D66
H	65	B69	60	A68	57	D67
H	68	B70	64	A69	59	D68

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B45	1.09243080
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D67	179.63605646
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Alkoxyamine 5

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C	1	B1		
C	1	B2	2	A1
H	1	B3	2	A2 3 D1
C	2	B4	1	A3 3 D2
C	3	B5	1	A4 2 D3
H	2	B6	1	A5 3 D4
H	3	B7	1	A6 2 D5
C	5	B8	2	A7 1 D6
C	6	B9	3	A8 1 D7
H	5	B10	2	A9 1 D8
O	10	B11	6	A10 3 D9
C	10	B12	6	A11 3 D10
H	9	B13	5	A12 2 D11
C	13	B14	10	A13 6 D12
C	13	B15	10	A14 6 D13
C	15	B16	13	A15 10 D14
C	16	B17	13	A16 10 D15
H	15	B18	13	A17 10 D16
H	16	B19	13	A18 10 D17
C	17	B20	15	A19 13 D18
H	17	B21	15	A20 13 D19
H	18	B22	16	A21 13 D20
N	21	B23	17	A22 15 D21
C	24	B24	21	A23 17 D22
H	24	B25	21	A24 17 D23
O	25	B26	24	A25 21 D24
C	25	B27	24	A26 21 D25
C	28	B28	25	A27 24 D26
O	28	B29	25	A28 24 D27
H	28	B30	25	A29 24 D28

C	29	B31	28	A30	25	D29
N	30	B32	28	A31	25	D30
H	29	B33	28	A32	25	D31
H	29	B34	28	A33	25	D32
C	32	B35	29	A34	28	D33
C	32	B36	29	A35	28	D34
C	32	B37	29	A36	28	D35
C	33	B38	30	A37	28	D36
C	33	B39	30	A38	28	D37
O	38	B40	32	A39	29	D38
O	38	B41	32	A40	29	D39
C	39	B42	33	A41	30	D40
C	39	B43	33	A42	30	D41
C	39	B44	33	A43	30	D42
P	40	B45	33	A44	30	D43
C	40	B46	33	A45	30	D44
H	36	B47	32	A46	29	D45
H	36	B48	32	A47	29	D46
H	36	B49	32	A48	29	D47
H	37	B50	32	A49	29	D48
H	37	B51	32	A50	29	D49
H	37	B52	32	A51	29	D50
H	40	B53	33	A52	30	D51
C	47	B54	40	A53	33	D52
C	47	B55	40	A54	33	D53
C	47	B56	40	A55	33	D54
O	46	B57	40	A56	33	D55
O	46	B58	40	A57	33	D56
O	46	B59	40	A58	33	D57
H	42	B60	38	A59	32	D58
H	43	B61	39	A60	33	D59
H	43	B62	39	A61	33	D60
H	43	B63	39	A62	33	D61
H	44	B64	39	A63	33	D62
H	44	B65	39	A64	33	D63
H	44	B66	39	A65	33	D64
H	45	B67	39	A66	33	D65
H	45	B68	39	A67	33	D66
H	45	B69	39	A68	33	D67
C	59	B70	46	A69	40	D68
C	60	B71	46	A70	40	D69
H	55	B72	47	A71	40	D70
H	55	B73	47	A72	40	D71
H	55	B74	47	A73	40	D72
H	56	B75	47	A74	40	D73
H	56	B76	47	A75	40	D74
H	56	B77	47	A76	40	D75
H	57	B78	47	A77	40	D76
H	57	B79	47	A78	40	D77
H	57	B80	47	A79	40	D78
C	71	B81	59	A80	46	D79
C	72	B82	60	A81	46	D80
H	71	B83	59	A82	46	D81

H	71	B84	59	A83	46	D82
H	72	B85	60	A84	46	D83
H	72	B86	60	A85	46	D84
H	82	B87	71	A86	59	D85
H	82	B88	71	A87	59	D86
H	82	B89	71	A88	59	D87
H	83	B90	72	A89	60	D88
H	83	B91	72	A90	60	D89
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B51	1.09579217
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B56	1.54200436
B57	1.48905691
B58	1.62188383
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B91	1.09474878
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D84	65.26562997
D85	-179.58567112
D86	-60.00795718
D87	60.61255101
D88	-179.11954951
D89	-59.35226216
D90	61.16677825

Alkoxyamine 6

C						
C	1	B1				
C	1	B2	2	A1		
H	1	B3	3	A2	2	D1
C	2	B4	1	A3	3	D2
C	3	B5	1	A4	2	D3
H	2	B6	1	A5	3	D4
H	3	B7	1	A6	2	D5
C	5	B8	2	A7	1	D6
C	6	B9	3	A8	1	D7
H	5	B10	2	A9	1	D8
O	10	B11	6	A10	3	D9
C	10	B12	6	A11	3	D10
H	9	B13	5	A12	2	D11
C	13	B14	10	A13	6	D12
C	13	B15	10	A14	6	D13
C	15	B16	13	A15	10	D14
C	16	B17	13	A16	10	D15
H	15	B18	13	A17	10	D16
H	16	B19	13	A18	10	D17
C	18	B20	16	A19	13	D18
H	17	B21	15	A20	13	D19
H	18	B22	16	A21	13	D20
O	21	B23	18	A22	16	D21
C	24	B24	21	A23	18	D22
O	25	B25	24	A24	21	D23
C	25	B26	24	A25	21	D24
C	27	B27	25	A26	24	D25
O	27	B28	25	A27	24	D26
H	27	B29	25	A28	24	D27
C	28	B30	27	A29	25	D28

N	29	B31	27	A30	25	D29
H	28	B32	27	A31	25	D30
H	28	B33	27	A32	25	D31
C	31	B34	28	A33	27	D32
C	31	B35	28	A34	27	D33
C	31	B36	28	A35	27	D34
C	32	B37	29	A36	27	D35
C	32	B38	29	A37	27	D36
O	37	B39	31	A38	28	D37
O	37	B40	31	A39	28	D38
C	38	B41	32	A40	29	D39
C	38	B42	32	A41	29	D40
C	38	B43	32	A42	29	D41
P	39	B44	32	A43	29	D42
C	39	B45	32	A44	29	D43
H	35	B46	31	A45	28	D44
H	35	B47	31	A46	28	D45
H	35	B48	31	A47	28	D46
H	36	B49	31	A48	28	D47
H	36	B50	31	A49	28	D48
H	36	B51	31	A50	28	D49
H	39	B52	32	A51	29	D50
C	46	B53	39	A52	32	D51
C	46	B54	39	A53	32	D52
C	46	B55	39	A54	32	D53
O	45	B56	39	A55	32	D54
O	45	B57	39	A56	32	D55
O	45	B58	39	A57	32	D56
H	41	B59	37	A58	31	D57
H	42	B60	38	A59	32	D58
H	42	B61	38	A60	32	D59
H	42	B62	38	A61	32	D60
H	43	B63	38	A62	32	D61
H	43	B64	38	A63	32	D62
H	43	B65	38	A64	32	D63
H	44	B66	38	A65	32	D64
H	44	B67	38	A66	32	D65
H	44	B68	38	A67	32	D66
C	58	B69	45	A68	39	D67
C	59	B70	45	A69	39	D68
H	54	B71	46	A70	39	D69
H	54	B72	46	A71	39	D70
H	54	B73	46	A72	39	D71
H	55	B74	46	A73	39	D72
H	55	B75	46	A74	39	D73
H	55	B76	46	A75	39	D74
H	56	B77	46	A76	39	D75
H	56	B78	46	A77	39	D76
H	56	B79	46	A78	39	D77
C	70	B80	58	A79	45	D78
C	71	B81	59	A80	45	D79
H	70	B82	58	A81	45	D80
H	70	B83	58	A82	45	D81

H	71	B84	59	A83	45	D82
H	71	B85	59	A84	45	D83
H	81	B86	70	A85	58	D84
H	81	B87	70	A86	58	D85
H	81	B88	70	A87	58	D86
H	82	B89	71	A88	59	D87
H	82	B90	71	A89	59	D88
H	82	B91	71	A90	59	D89

B1	1.39547682
B2	1.39546500
B3	1.08655342
B4	1.39842474
B5	1.40352627
B6	1.08685449
B7	1.08522780
B8	1.39131133
B9	1.50038094
B10	1.08667215
B11	1.22686205
B12	1.50007348
B13	1.08522197
B14	1.40442070
B15	1.40368850
B16	1.38992668
B17	1.39529040
B18	1.08505060
B19	1.08484300
B20	1.39209382
B21	1.08500547
B22	1.08677407
B23	1.40302429
B24	1.36299139
B25	1.20818698
B26	1.53354107
B27	1.54360102
B28	1.43022750
B29	1.09096098
B30	1.55345769
B31	1.45182433
B32	1.09362034
B33	1.09620114
B34	1.55138167
B35	1.53812135
B36	1.53114277
B37	1.50069205
B38	1.48501026
B39	1.20908996
B40	1.36139303
B41	1.53731006
B42	1.54526861
B43	1.54421000
B44	1.87806016

B45	1.59103623
B46	1.09527814
B47	1.09430533
B48	1.09594829
B49	1.09288716
B50	1.09592911
B51	1.09357238
B52	1.09174658
B53	1.55044807
B54	1.54132946
B55	1.54520747
B56	1.49338447
B57	1.62200089
B58	1.61839626
B59	0.97616847
B60	1.09553541
B61	1.09008218
B62	1.09148595
B63	1.09564389
B64	1.09445980
B65	1.09420486
B66	1.09615133
B67	1.09265808
B68	1.09099349
B69	1.45367595
B70	1.45119138
B71	1.09623334
B72	1.09507688
B73	1.09322416
B74	1.09705597
B75	1.09201061
B76	1.09182583
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B78	1.09118150
B79	1.09440538
B80	1.51740694
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B82	1.09319924
B83	1.09322956
B84	1.09499873
B85	1.09538319
B86	1.09577781
B87	1.09509532
B88	1.09514706
B89	1.09580447
B90	1.09474254
B91	1.09455868
A1	120.10982714
A2	119.73106439
A3	119.94613456
A4	120.30122822
A5	120.01764578
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A7	120.01016083
A8	123.09494063
A9	120.06098646
A10	119.70157166
A11	120.68482405
A12	121.08119182
A13	117.60617440
A14	123.34172182
A15	120.65073089
A16	121.13883458
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A18	120.11323289
A19	118.33895232
A20	121.67350031
A21	120.62425823
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A23	118.94645102
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A25	111.83208889
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A27	113.57988262
A28	105.69659523
A29	117.91829904
A30	111.85942176
A31	108.74395224
A32	105.61945154
A33	107.33939264
A34	111.98755452
A35	113.07281874
A36	107.64240535
A37	107.74842551
A38	125.61815729
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A40	109.82144039
A41	106.70543339
A42	114.54795453
A43	110.19470123
A44	125.35939212
A45	110.72264517
A46	111.42397613
A47	109.78171837
A48	110.46178030
A49	110.00070342
A50	112.02287336
A51	100.58576936
A52	107.37568433
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A54	108.41606027
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A56	109.53276681
A57	105.50483908
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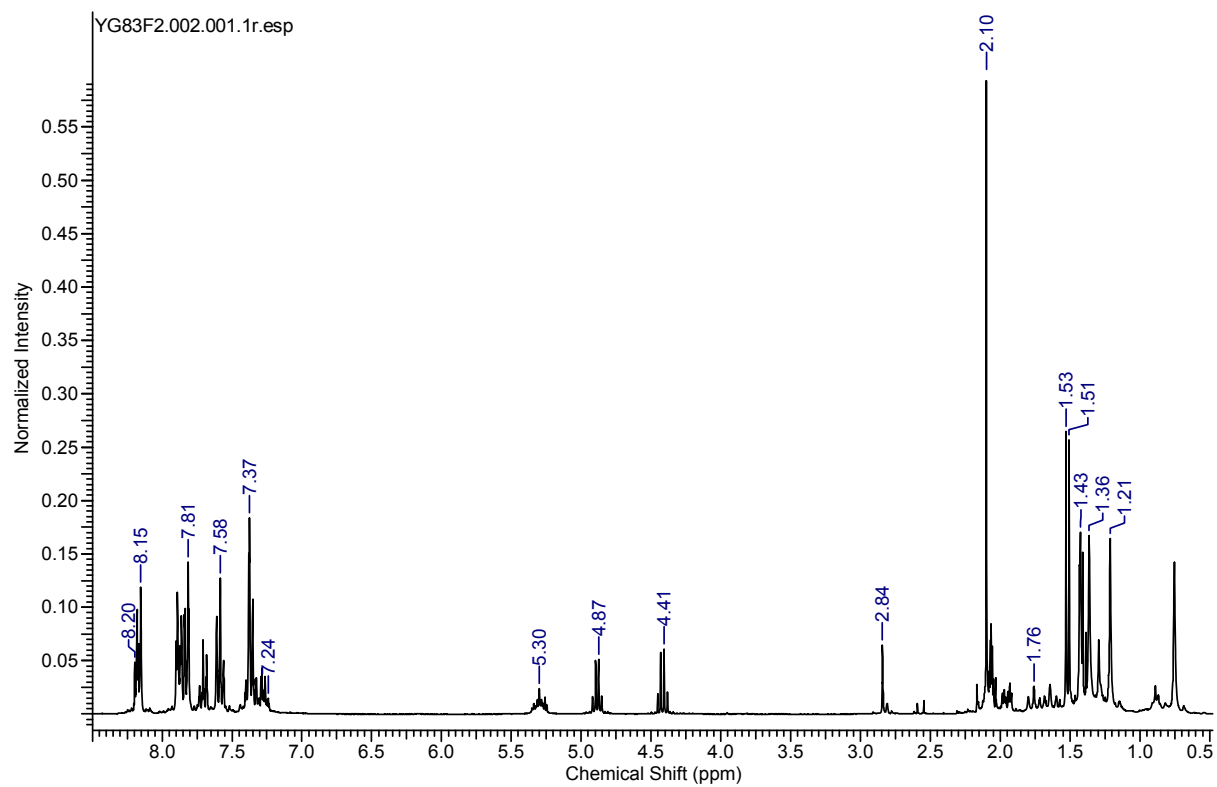
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A71	111.98527669
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A86	111.02385309
A87	111.01330296
A88	109.82737207
A89	110.81152831
A90	110.81181693
D1	179.87706436
D2	0.95996719
D3	-0.61282111
D4	-179.42708765
D5	-179.01759135
D6	-0.00752986
D7	-176.66069487
D8	179.59170167
D9	149.82401106
D10	-30.04134374
D11	178.61092280
D12	154.77514277
D13	-29.38147268
D14	178.00689257
D15	-176.81199234
D16	-1.76648147
D17	1.36187755
D18	-0.62834441
D19	179.26323775
D20	178.44329756
D21	177.08926011
D22	70.88659228

D23	-2.78530898
D24	174.95126332
D25	-72.37934825
D26	46.21895724
D27	166.42905116
D28	-76.19202394
D29	77.03325056
D30	49.92396769
D31	164.26167508
D32	-179.55186756
D33	-59.58540715
D34	63.52406056
D35	112.90721882
D36	-106.96323743
D37	-139.89669309
D38	43.11894756
D39	173.08820002
D40	-70.84070592
D41	48.14269780
D42	140.06206663
D43	-73.04342588
D44	-179.32890774
D45	-58.57105539
D46	61.47542735
D47	-174.76314937
D48	-54.94922835
D49	66.01244584
D50	38.94191091
D51	165.53072946
D52	-74.03806408
D53	50.29093456
D54	-128.88413490
D55	-3.12669742
D56	104.71787830
D57	-178.96739451
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D59	-62.29353767
D60	59.85117202
D61	-173.91144394
D62	-54.48118019
D63	67.12980908
D64	-171.68959837
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D67	-100.69848489
D68	178.50769283
D69	-172.01728931
D70	-52.81730917
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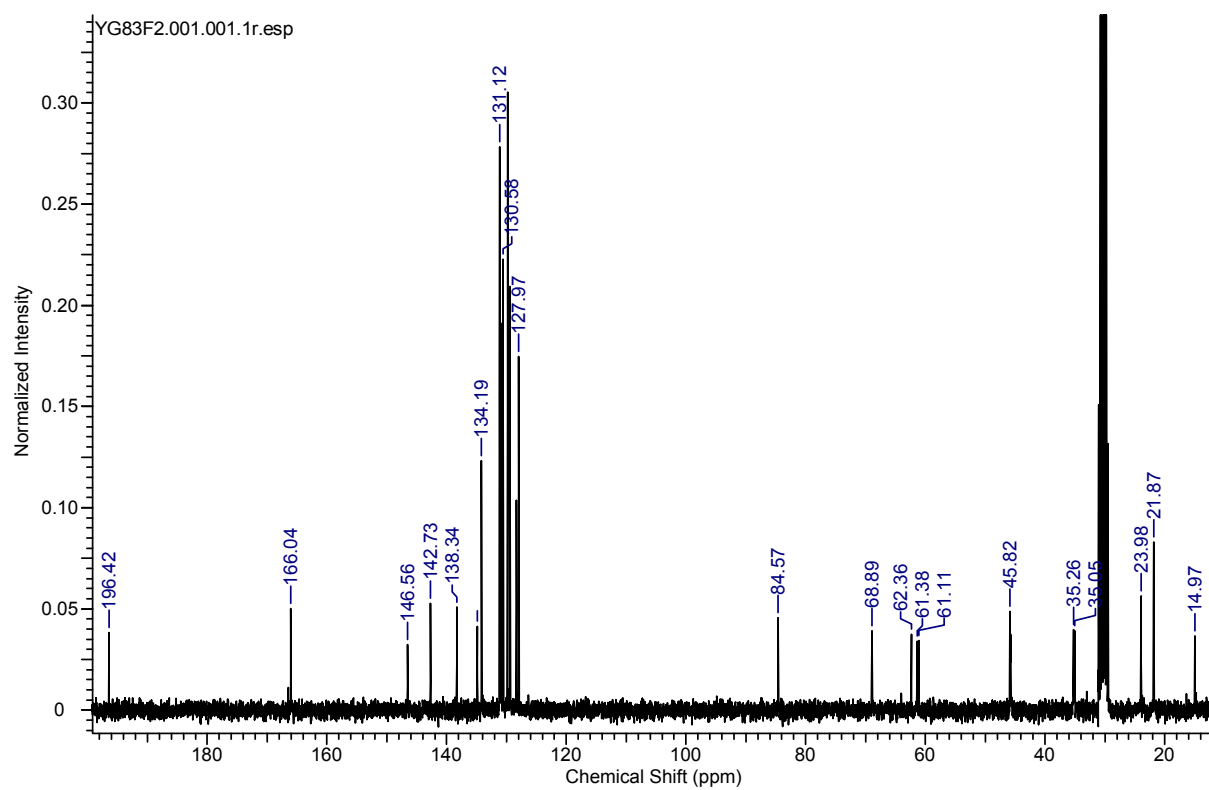
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D78	-160.60254741
D79	-169.24528875
D80	-39.29214628
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D82	-48.05669854
D83	69.88760025
D84	-179.21300500
D85	-59.60021163
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D88	-59.17639101
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Alkoxyamine 4

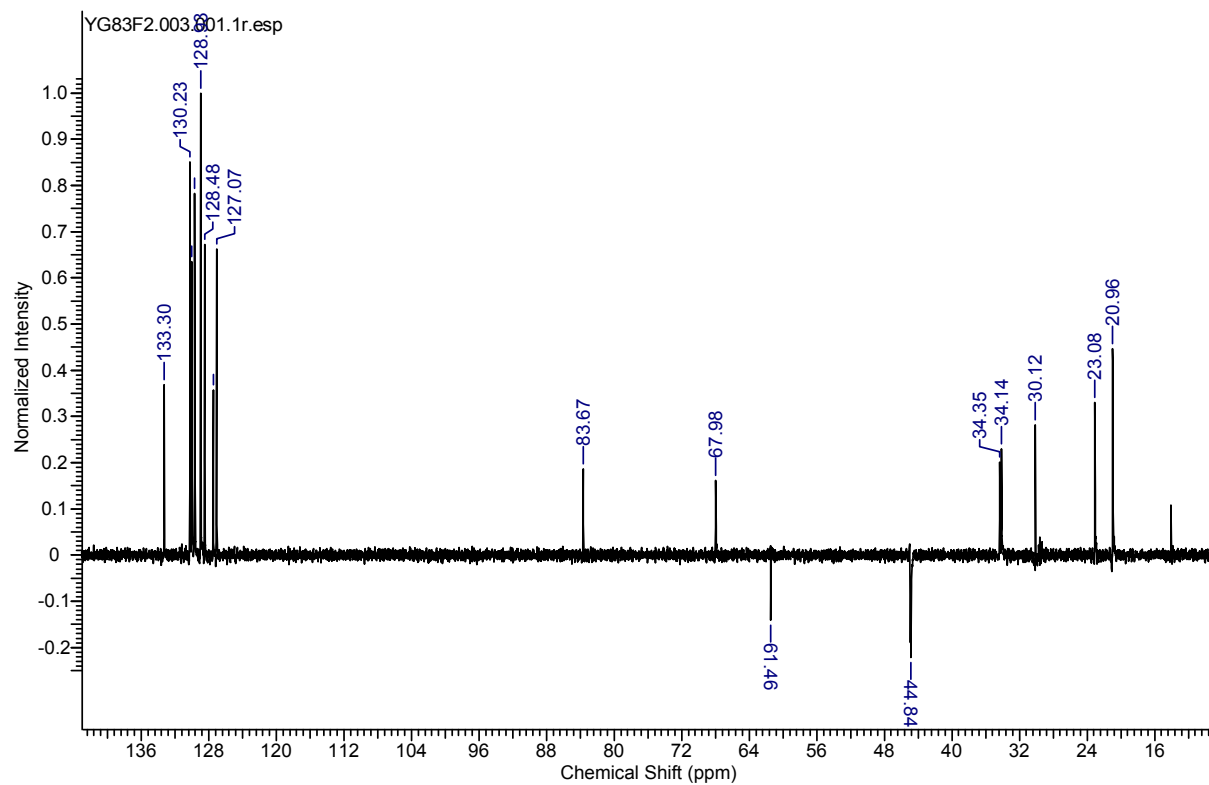
^1H NMR



^{13}C NMR

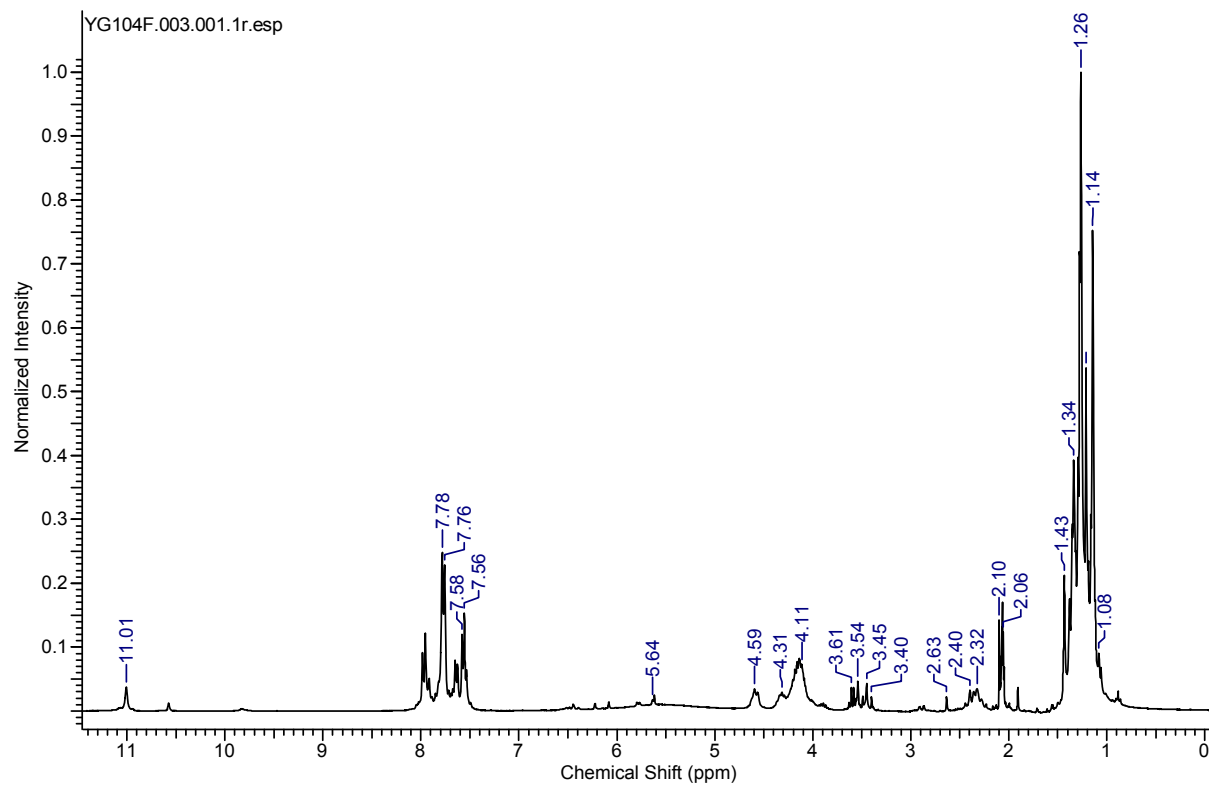


¹³C DEPT NMR

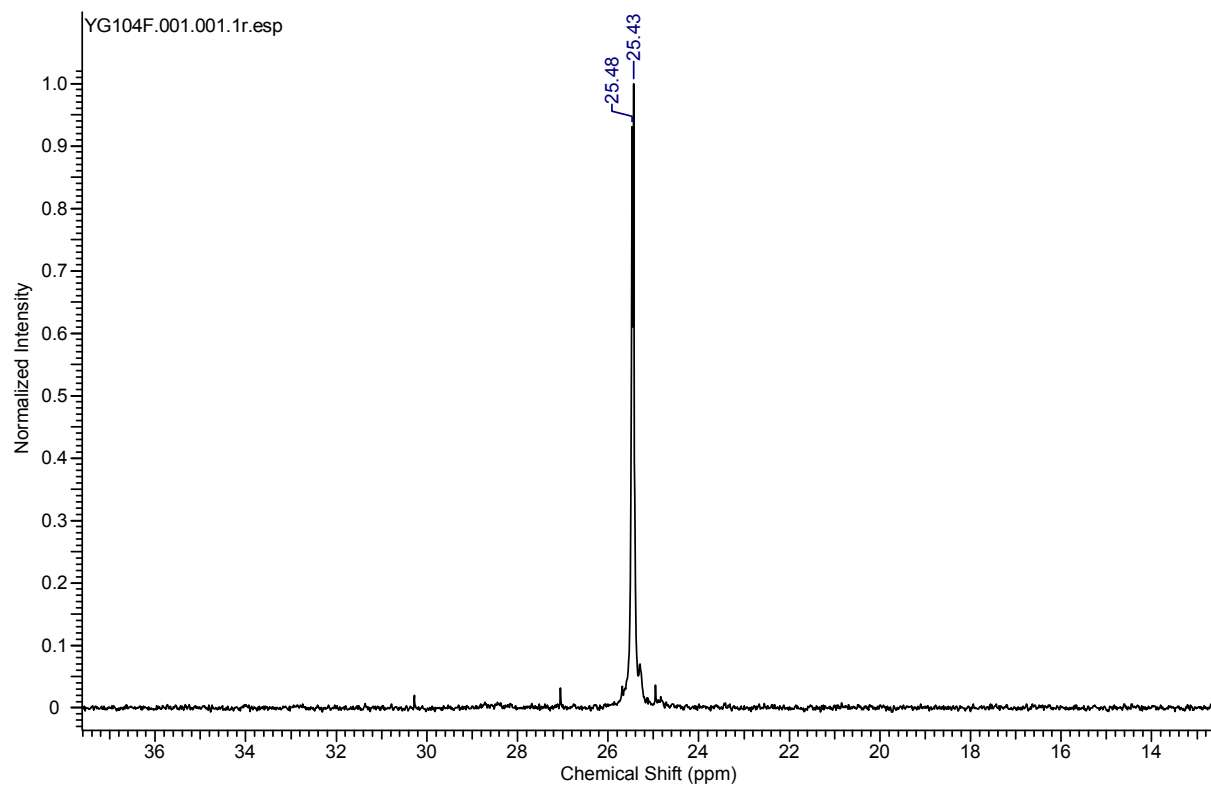


Alkoxyamine 5

^1H NMR

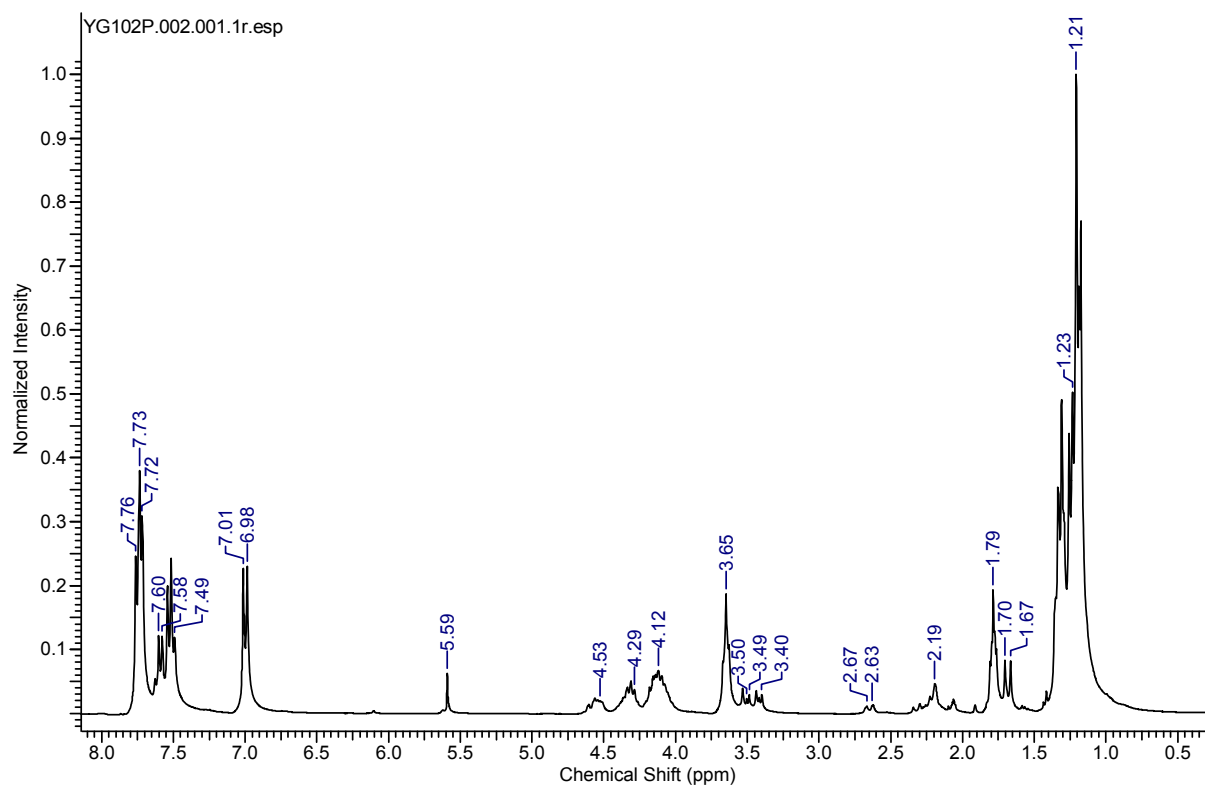


^{31}P NMR



Alkoxyamine 6

^1H NMR



^{31}P NMR

