

APPENDIX A

The input file of the reaction

The input file of the reaction between glyceride and methoxide

Example: The reaction between monoolein and methoxide

%chk=Triolein add 1 Methoxide with -1 charge 1 spin.chk

%mem=6MW

%nproc=1

opt hf/6-31g geom=connectivity

Title Card Required

-1 1

O

C	1	B1			
H	2	B2	1	A1	
H	2	B3	1	A2	3 D1
C	1	B4	2	A3	3 D2
H	5	B5	1	A4	2 D3
H	5	B6	1	A5	2 D4
O	2	B7	1	A6	5 D5
C	8	B8	2	A7	1 D6
O	9	B9	8	A8	2 D7
C	9	B10	8	A9	2 D8
H	11	B11	9	A10	8 D9
H	11	B12	9	A11	8 D10
C	11	B13	9	A12	8 D11
H	14	B14	11	A13	9 D12
H	14	B15	11	A14	9 D13
C	14	B16	11	A15	9 D14
H	17	B17	14	A16	11 D15
H	17	B18	14	A17	11 D16
C	17	B19	14	A18	11 D17
H	20	B20	17	A19	14 D18

H	20	B21	17	A20	14	D19
C	20	B22	17	A21	14	D20
H	23	B23	20	A22	17	D21
H	23	B24	20	A23	17	D22
C	23	B25	20	A24	17	D23
H	26	B26	23	A25	20	D24
H	26	B27	23	A26	20	D25
C	26	B28	23	A27	20	D26
H	29	B29	26	A28	23	D27
H	29	B30	26	A29	23	D28
C	29	B31	26	A30	23	D29
H	32	B32	29	A31	26	D30
C	32	B33	29	A32	26	D31
H	34	B34	32	A33	29	D32
C	34	B35	32	A34	29	D33
H	36	B36	34	A35	32	D34
H	36	B37	34	A36	32	D35
C	36	B38	34	A37	32	D36
H	39	B39	36	A38	34	D37
H	39	B40	36	A39	34	D38
C	39	B41	36	A40	34	D39
H	42	B42	39	A41	36	D40
H	42	B43	39	A42	36	D41
C	42	B44	39	A43	36	D42
H	45	B45	42	A44	39	D43
H	45	B46	42	A45	39	D44
C	45	B47	42	A46	39	D45
H	48	B48	45	A47	42	D46
H	48	B49	45	A48	42	D47
C	48	B50	45	A49	42	D48
H	51	B51	48	A50	45	D49
H	51	B52	48	A51	45	D50

C	51	B53	48	A52	45	D51
H	54	B54	51	A53	48	D52
H	54	B55	51	A54	48	D53
C	54	B56	51	A55	48	D54
H	57	B57	54	A56	51	D55
H	57	B58	54	A57	51	D56
H	57	B59	54	A58	51	D57
O	5	B60	1	A59	2	D58
C	1	B61	2	A60	8	D59
H	62	B62	1	A61	2	D60
H	61	B63	5	A62	1	D61
O	11	B64	9	A63	8	D62
C	65	B65	11	A64	9	D63
H	66	B66	65	A65	11	D64
H	66	B67	65	A66	11	D65
H	66	B68	65	A67	11	D66
H	1	B69	62	A68	5	D67

B1	2.46130200
B2	1.11987721
B3	1.12278827
B4	2.48154337
B5	1.12435238
B6	1.12512669
B7	1.43300877
B8	1.36911129
B9	1.23563855
B10	1.48860550
B11	1.14813732
B12	1.11890448
B13	1.51598956
B14	1.12121999

B15	1.11944390
B16	1.51530868
B17	1.12680884
B18	1.12175195
B19	1.51461269
B20	1.12127413
B21	1.12081804
B22	1.51480576
B23	1.12231262
B24	1.12172889
B25	1.51547752
B26	1.12094876
B27	1.12051599
B28	1.51736107
B29	1.12538234
B30	1.12443114
B31	1.48057847
B32	1.10171561
B33	1.33854116
B34	1.10016247
B35	1.48156847
B36	1.12461437
B37	1.12518971
B38	1.51635170
B39	1.12122069
B40	1.12095773
B41	1.51562349
B42	1.12193340
B43	1.12169658
B44	1.51418803
B45	1.12123564
B46	1.12144118

B47	1.51499295
B48	1.12168471
B49	1.12176348
B50	1.51445062
B51	1.12138689
B52	1.12143326
B53	1.51516800
B54	1.12182336
B55	1.12188967
B56	1.50795197
B57	1.11677918
B58	1.11699569
B59	1.11679616
B60	1.40815883
B61	1.43301736
B62	1.12936803
B63	0.96000000
B64	2.14763525
B65	1.36702000
B66	1.07000000
B67	1.07000000
B68	1.07000000
B69	0.96000000
A1	83.01089246
A2	138.37646433
A3	61.09309714
A4	141.38573317
A5	90.81027913
A6	103.57542555
A7	117.26639407
A8	117.94184107
A9	113.48429914

A10	108.07705593
A11	109.90045645
A12	111.56668989
A13	108.55713682
A14	111.17976367
A15	109.08835429
A16	107.74226786
A17	109.66913279
A18	112.12469884
A19	109.18488941
A20	110.20823832
A21	110.19136890
A22	109.12722002
A23	109.36431676
A24	112.30660532
A25	109.61802933
A26	109.85182299
A27	110.17444966
A28	109.21588489
A29	108.90889476
A30	113.24042185
A31	115.79069656
A32	123.68880389
A33	120.72735417
A34	123.12452307
A35	109.70833490
A36	108.82964894
A37	112.97600433
A38	109.88273753
A39	109.74823416
A40	110.31568275
A41	109.36086350

A42	109.46851815
A43	111.79515720
A44	109.63751687
A45	109.69709300
A46	110.82517081
A47	109.49675904
A48	109.47089065
A49	111.51823718
A50	109.58794829
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A52	111.14595087
A53	109.39422545
A54	109.38905077
A55	111.58548209
A56	110.62088238
A57	110.34555206
A58	110.63817693
A59	92.29648568
A60	35.28471403
A61	101.01570415
A62	109.47122063
A63	44.90745982
A64	136.13366866
A65	109.47120255
A66	109.47120255
A67	109.47123134
A68	109.47122063
D1	111.68361226
D2	-119.79257247
D3	-29.89514654
D4	94.04105612
D5	132.19363311

D6	145.54228149
D7	-0.93053245
D8	-179.61687640
D9	-103.89601008
D10	15.17113345
D11	138.53802026
D12	69.61901277
D13	-49.56730107
D14	-171.85889449
D15	-51.82021252
D16	65.97156261
D17	-172.39087000
D18	64.35393949
D19	-53.59875988
D20	-174.49586872
D21	-52.96230534
D22	64.15182190
D23	-174.10687637
D24	61.59594182
D25	-56.18678125
D26	-177.07004712
D27	-55.80259599
D28	60.49130912
D29	-176.67819007
D30	21.08553487
D31	-159.66473844
D32	-178.81515085
D33	1.80238120
D34	-47.42642263
D35	68.94774316
D36	-169.48470288
D37	-56.02719859

D38	61.79880276
D39	-177.04488590
D40	60.93542439
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D43	61.25583227
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D46	-56.34427141
D47	60.85396244
D48	-177.70945276
D49	59.98378544
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D51	-178.74686447
D52	-57.16682239
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D54	-178.61603427
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D56	-179.43982399
D57	-59.40671654
D58	-158.77834440
D59	100.30342717
D60	-117.46558903
D61	148.43089333
D62	-90.50651363
D63	-180.00000000
D64	85.36436622
D65	-154.63561898
D66	-34.63562638
D67	125.30467425

2 3 1.0 4 1.0 8 1.0 62 1.0

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5 6 1.0 7 1.0 61 1.0 62 1.0

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9 10 2.0 11 1.0

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14 15 1.0 16 1.0 17 1.0

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34 35 1.0 36 1.0

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