Intramolecular Heck Insertion of a Diene-Allylic Amination Cascade to Synthesize a 2-Alkenyl-3,4-Fused Indole Structure

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Supporting Information

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1. Computational Details

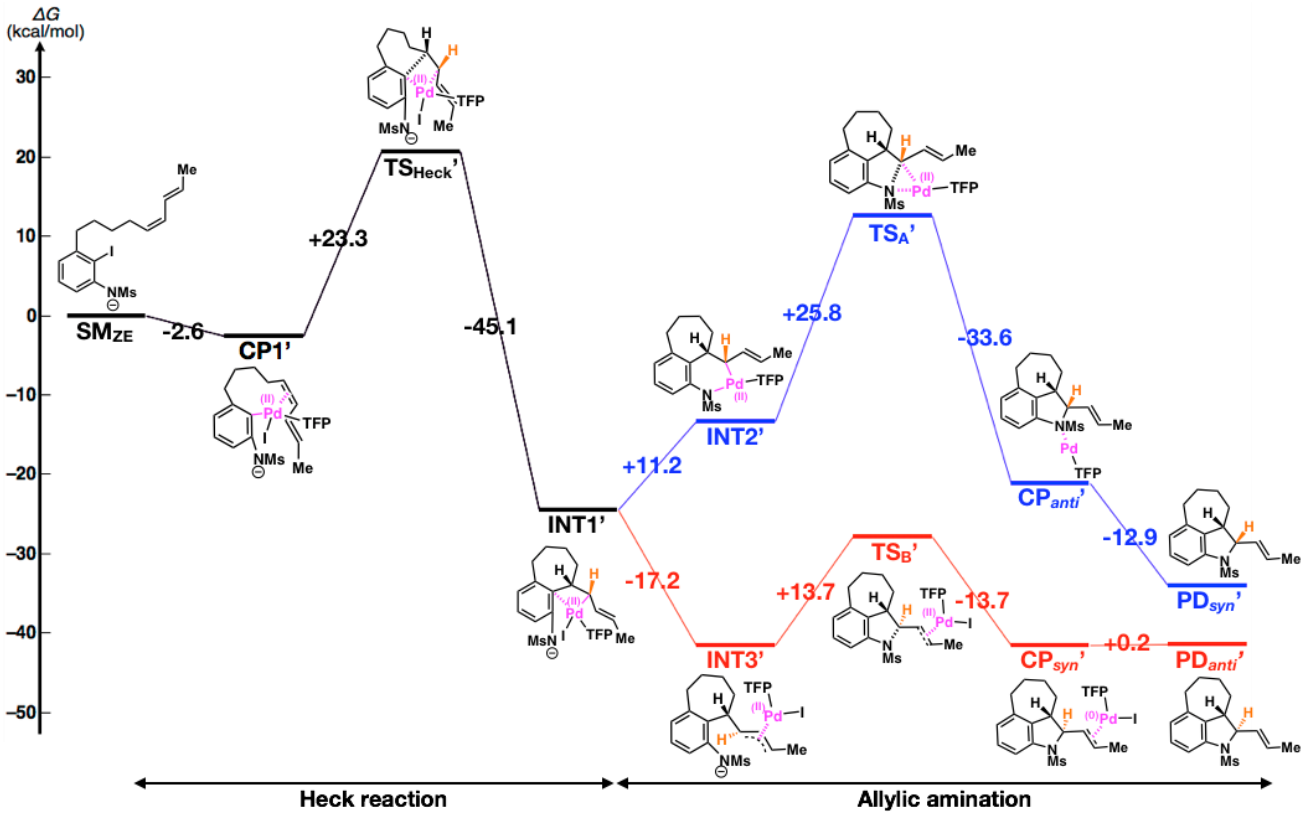
1-1. General

All calculations were carried with the Gaussian 16 program package.[1)] The molecular structures and harmonic vibrational frequencies were obtained using the hybrid density functional method based on B3LYP functional. We used LANL2DZ basis set for Pd and I atoms and 6–31+G* for the other atoms. Geometry optimization and vibrational analysis were performed at the same level. Single point energies were calculated using B3LYP functional with SDD for Pd and I and 6-311++G** for the other atoms.

All stationary points were optimized without any symmetry assumptions and characterized by normal coordinate analysis at the same level of theory. The number of imaginary frequencies was comfirmed 0 for minima and 1 for TSs. The intrinsic reaction coordinate (IRC) method was used to track minimum energy paths from transition structures to the corresponding local minima.

1) Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

1-2. Energy Profiles from a (Z,E)-Diene Substrate



DFT-computed pathways for the Heck reaction and allylic amination. Optimization of geometries and frequencies are computed at the B3LYP/LanL2DZ (for Pd, I), 6-31+G* (others) levels, and single point energies are computed at the B3LYP/SDD (for Pd, I), 6-311++G** (others) levels.

1-3. Cartesian Coordinates and Computed Energies

SM$_{EE}$

B3LYP/6-31+G*/LanL2DZ, E= -1237.113101 A.U.

Thermal correction to Gibbs Free Energy = 0.284348 A.U.

SP at B3LYP/6-311++G**/SDD, E= -1237.383391 A.U.

-1 1

C -1.00942 -0.99308 -3.06329
C 0.10566 -1.29736 -2.29274
C 0.05743 -1.27213 -0.86799
C -1.21286 -0.92740 -0.30590
C -2.33072 -0.56636 -1.06642
C -2.21864 -0.62816 -2.46962
N 1.09265 -1.55554 -0.02552
I -1.30860 -0.99747 1.85919
C -3.63526 -0.04172 -0.49270
C -3.84136 1.48962 -0.64280
C -2.72706 2.37958 -0.04439
C -1.59597 2.71638 -1.04518
C -0.41999 3.41625 -0.42007
C 0.81208 2.87699 -0.33242
C 1.97114 3.51769 0.27471
C 3.18446 2.93678 0.35426
C 4.39549 3.57233 0.97549
C 3.39290 -2.17675 1.01075
S 2.60882 -1.70964 -0.55053
O 2.85370 -2.84001 -1.49644
O 3.23737 -0.41559 -0.96169
H -0.93079 -1.03727 -4.14866
H 1.03602 -1.58203 -2.77193
H -3.07932 -0.36357 -3.08129
H -3.71762 -0.30298 0.56550
H -4.47077 -0.54148 -1.00465
H -4.80043 1.73077 -0.15982
H -3.96662 1.73774 -1.70747
H -2.29393 1.88799 0.83469
H -3.16822 3.32199 0.31516
H -2.02511 3.34427 -1.84476
H -1.24771 1.79744 -1.52497
H -0.59747 4.41128 0.00025
H 0.98085 1.87824 -0.73714
H 1.82681 4.52276 0.68237
H 3.30995 1.93005 -0.04932
H 4.17871 4.57916 1.35566
H 5.21992 3.65132 0.25127
H 4.77706 2.96761 1.81165
H 3.22280 -1.38321 1.74071
H 4.45959 -2.29574 0.80310
H 2.95653 -3.11652 1.35463

CP1

B3LYP/6-31+G*/LanL2DZ, E= -2393.566352 A.U.

Thermal correction to Gibbs Free Energy= 0.447234 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.217197 A.U.

-1 1

C -5.13766 -0.16393 -0.72426
C -4.30473 0.95569 -0.78129
C -2.94950 0.86443 -0.37797
C -2.49270 -0.41021 0.04966
C -3.33993 -1.49846 0.22159
C -4.67739 -1.37433 -0.21043
N -2.00458 1.88870 -0.31228
Pd -0.47679 -0.36738 0.31403
P 2.03854 0.06232 0.00015
I -0.39246 -2.03877 -1.90898
C 3.17548 -0.70249 1.21428
C 4.44740 -0.46741 1.66559
C 4.74711 -1.49652 2.61504
C 3.63897 -2.29307 2.67095
O 2.67778 -1.82685 1.83420
C 2.46904 1.82234 0.03450
C 2.87989 -0.41003 -1.55854
C 2.52269 4.06382 -0.06632
C 3.79666 3.58303 0.00968
O 3.79531 2.22171 0.06566
O 3.38028 -1.68081 -1.65506
C 3.87530 -1.82714 -2.91447
C 3.71200 -0.67531 -3.62643
C 3.06358 0.24907 -2.74401
C 1.65804 2.92090 -0.04983
C -2.94465 -2.75102 0.98251
C -3.67338 -2.81812 2.34822
C -3.20011 -1.84934 3.45795
C -2.72136 -0.43593 3.06060
C -1.25323 -0.38932 2.66699
C -0.52197 0.76735 2.47751
C 0.81759 0.84628 3.05934
C 1.41794 1.97497 3.47537
C 2.70200 2.00279 4.25477
C -2.27195 3.23941 -2.69155
S -2.31065 3.36094 -0.87095
O -3.65391 3.92345 -0.54775
O -1.14821 4.21972 -0.50893
H -6.17027 -0.07420 -1.05803
H -4.70408 1.91393 -1.09439
H -5.35005 -2.22631 -0.12249
H 5.08432 0.34570 1.34887
H 5.66327 -1.62713 3.17603
H 3.38664 -3.18572 3.22415
H 2.21450 5.09864 -0.12767
H 4.77192 4.04827 0.03325
H 4.29897 -2.79421 -3.14031
H 4.00589 -0.50473 -4.65362
H 2.75838 1.26336 -2.96078
H 0.57465 2.94597 -0.10159
H -1.85833 -2.79572 1.10891
H -3.22575 -3.64160 0.40266
H -3.59795 -3.84165 2.74666
H -4.74064 -2.64430 2.16156
H -2.38109 -2.32290 4.02166
H -4.02373 -1.74191 4.17806
H -2.78682 0.18848 3.96845
H -3.37466 0.03734 2.32282
H -0.68349 -1.25977 2.99537
H -1.03744 1.69686 2.23760
H 1.28836 -0.10986 3.29031
H 0.94966 2.93633 3.26082
H 3.10219 0.99290 4.40378
H 2.55556 2.46239 5.24427
H 3.47063 2.59914 3.74117
H -1.27571 2.90595 -2.98996
H -2.49126 4.22918 -3.10179
H -3.02616 2.51613 -3.01313

TS_{Heck}

B3LYP/6-31+G*/LanL2DZ, E= -2393.523961 A.U.

Thermal correction to Gibbs Free Energy= 0.448088 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.174271 A.U.

Imaginary frequency -308.5935 cm^{-1}

-1 1

C -5.03943 -0.29319 -0.84301
C -4.24228 0.84604 -0.80781
C -2.92242 0.80148 -0.28314
C -2.47577 -0.45564 0.24680
C -3.31119 -1.57890 0.27357
C -4.58486 -1.50089 -0.31118
N -2.01755 1.84983 -0.26934
Pd -0.34502 -0.39415 0.17402
P 2.01640 0.00186 -0.11585
I -0.39953 -2.13373 -2.02454
C 3.13299 -0.76993 1.11579
C 4.40574 -0.52852 1.56276
C 4.71569 -1.55940 2.50654
C 3.61215 -2.36211 2.56345
O 2.64524 -1.89900 1.73129
C 2.45407 1.75913 -0.06314
C 2.87182 -0.47627 -1.66181
C 2.52168 4.00070 -0.14549
C 3.79275 3.51100 -0.07801
O 3.78252 2.14958 -0.03248
O 3.37161 -1.74749 -1.74906
C 3.87366 -1.89963 -3.00424
C 3.71736 -0.75030 -3.72218
C 3.06477 0.17839 -2.84808
C 1.64977 2.86345 -0.13522
C -2.98417 -2.83237 1.06014
C -3.72640 -2.81562 2.42035
C -3.24595 -1.78599 3.46969
C -2.85724 -0.37197 2.98222
C -1.52151 -0.40180 2.22742
C -0.60571 0.69126 2.14356
C 0.63642 0.65728 2.91319
C 1.28303 1.75318 3.36109
C 2.52227 1.73300 4.20985
C -2.26437 3.06515 -2.72583
S -2.33602 3.28743 -0.91649
O -3.68849 3.85338 -0.64276
O -1.18466 4.17199 -0.58767
H -6.03568 -0.23222 -1.27910
H -4.63058 1.78999 -1.17296
H -5.22478 -2.38208 -0.31825
H 5.03691 0.28925 1.24681
H 5.63436 -1.68573 3.06437
H 3.36590 -3.25725 3.11535
H 2.22085 5.03822 -0.19684
H 4.77106 3.96974 -0.05437
H 4.29543 -2.86884 -3.22427
H 4.01748 -0.58493 -4.74838
H 2.76150 1.19196 -3.07102
H 0.56671 2.89286 -0.18059
H -1.90380 -2.94986 1.18922
H -3.32314 -3.71186 0.49656
H -3.66570 -3.81450 2.87949
H -4.78946 -2.63823 2.21065
H -2.37075 -2.19764 3.99613
H -4.03055 -1.68713 4.23399
H -2.68138 0.24510 3.87868
H -3.66098 0.11196 2.42275
H -1.00550 -1.33911 2.45462
H -1.02398 1.67586 1.94521
H 1.01946 -0.32849 3.18310
H 0.89451 2.73559 3.08996
H 2.84502 0.70820 4.42754
H 2.36287 2.25168 5.16754
H 3.35641 2.24733 3.71002
H -1.26063 2.72570 -2.98971
H -2.48237 4.03294 -3.18585
H -3.00703 2.32174 -3.02636

INT1

B3LYP/6-31+G*/LanL2DZ, E= -2393.575728 A.U.

Thermal correction to Gibbs Free Energy= 0.450503 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.223412 A.U.

-1 1

C -4.92895 -0.25722 -0.85878
C -4.18923 0.90274 -0.71885
C -2.94243 0.91454 -0.02711
C -2.58283 -0.29124 0.71842
C -3.34506 -1.47374 0.49800
C -4.47970 -1.46349 -0.30742
N -2.06522 1.96943 -0.05871
Pd -0.22174 -0.30572 0.18438
P 2.01835 0.08529 -0.01924
I -0.39813 -2.07735 -1.95399
C 3.12121 -0.69310 1.21752
C 4.39670 -0.45068 1.65693
C 4.71427 -1.48587 2.59282
C 3.61191 -2.29029 2.65199
O 2.63953 -1.82537 1.82801
C 2.45777 1.84008 0.03572
C 2.87029 -0.39907 -1.56405
C 2.53352 4.08064 -0.05137
C 3.80285 3.58602 0.01402
O 3.78728 2.22504 0.06285
O 3.36896 -1.67069 -1.65050
C 3.87191 -1.82357 -2.90470
C 3.71847 -0.67388 -3.62334
C 3.06554 0.25512 -2.75077
C 1.65745 2.94712 -0.03736
C -3.07466 -2.74095 1.28444
C -3.76258 -2.68013 2.66812
C -3.16780 -1.69578 3.70464
C -2.83553 -0.25392 3.24803
C -1.79676 -0.27794 2.07683
C -0.64080 0.70535 2.05094
C 0.44917 0.63279 3.01948
C 1.15772 1.71555 3.41678
C 2.37130 1.70400 4.30181
C -2.25020 3.07504 -2.60168
S -2.35377 3.37078 -0.80407
O -3.70525 3.95206 -0.57076
O -1.19581 4.25402 -0.50296
H -5.86328 -0.22979 -1.41837
H -4.55709 1.83191 -1.13752
H -5.04311 -2.38207 -0.45862
H 5.02485 0.36924 1.34055
H 5.63607 -1.61292 3.14525
H 3.36946 -3.18740 3.20234
H 2.23740 5.11946 -0.10354
H 4.78288 4.04117 0.03460
H 4.29239 -2.79342 -3.12432
H 4.02003 -0.50930 -4.64922
H 2.76311 1.26877 -2.97457
H 0.57503 2.97983 -0.08041
H -2.00271 -2.94664 1.38042
H -3.49473 -3.58756 0.72712
H -3.74811 -3.68366 3.12111
H -4.82015 -2.43237 2.49887
H -2.23407 -2.13139 4.09403
H -3.85655 -1.65098 4.56187
H -2.41598 0.28772 4.10717
H -3.73553 0.28751 2.92947
H -1.31527 -1.26282 2.19104
H -0.92053 1.72151 1.79067
H 0.73450 -0.35294 3.39685
H 0.86157 2.68975 3.02622
H 2.62141 0.68888 4.63611
H 2.23073 2.33396 5.19443
H 3.24776 2.10562 3.76996
H -1.24725 2.71117 -2.83397
H -2.43950 4.03410 -3.09150
H -2.99958 2.33745 -2.89759

INT2

B3LYP/6-31+G*/LanL2DZ, E= -2382.087588 A.U.

Thermal correction to Gibbs Free Energy= 0.454802 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2383.702771 A.U.

0 1

C 4.45955 -1.27211 -2.50017
C 3.56889 -1.82187 -1.58598
C 2.83578 -1.00456 -0.70679
C 2.97938 0.40316 -0.75634
C 3.86958 0.95598 -1.71073
C 4.60034 0.11378 -2.55974
N 1.86862 -1.63984 0.12913
Pd 0.02576 -0.72049 0.06082
P -2.19448 -0.07185 -0.36394
C -3.26287 -0.23702 1.08548
C -2.99765 -0.80182 2.30649
C -4.20508 -0.70897 3.06835
C -5.11471 -0.08870 2.25995
O -4.56499 0.20457 1.05248
C -2.83331 -1.27580 -1.56451
C -2.74393 1.48420 -1.13644
C -3.15614 -2.89120 -3.09738
C -4.36064 -2.40363 -2.67913
O -4.18787 -1.42409 -1.75254
O -2.63500 2.63955 -0.40303
C -3.04619 3.66565 -1.20155
C -3.40609 3.19824 -2.43028
C -3.21080 1.77949 -2.38986
C -2.16311 -2.16008 -2.37117
C 4.08534 2.45298 -1.85058
C 4.78983 3.11490 -0.64803
C 3.87720 3.34435 0.56210
C 3.20172 2.09293 1.14048
C 2.21173 1.36535 0.15677
C 1.06191 0.83847 1.02712
C 0.07033 1.85126 1.41633
C -0.43609 1.96323 2.66206
C -1.42966 2.99484 3.10432
C 3.18709 -3.78926 1.27368
S 2.34390 -2.22364 1.61135
O 3.34211 -1.35251 2.27362
O 1.10601 -2.55593 2.34788
H 5.02136 -1.91332 -3.17513
H 3.39888 -2.89407 -1.55498
H 5.27843 0.55671 -3.28592
H -2.05172 -1.23028 2.61229
H -4.36999 -1.05258 4.08046
H -6.14529 0.20824 2.38876
H -2.99388 -3.67422 -3.82526
H -5.38581 -2.63736 -2.92657
H -3.02730 4.64626 -0.74981
H -3.77182 3.78534 -3.26165
H -3.39981 1.07087 -3.18370
H -1.08835 -2.26974 -2.43552
H 3.12846 2.96692 -2.02967
H 4.68969 2.62350 -2.74934
H 5.19199 4.08616 -0.96893
H 5.65243 2.49947 -0.35676
H 3.09550 4.06828 0.28225
H 4.45992 3.82187 1.36262
H 2.64130 2.40629 2.02904
H 3.94416 1.36323 1.48318
H 1.77518 2.13577 -0.49578
H 1.42778 0.29452 1.89828
H -0.24678 2.56078 0.65146
H -0.10928 1.24871 3.41971
H -1.70410 3.66986 2.28720
H -1.03100 3.59669 3.93325
H -2.34781 2.51836 3.47673
H 4.08519 -3.59421 0.68483
H 2.49867 -4.45087 0.74476
H 3.45728 -4.20916 2.24598

TS_A

B3LYP/6-31+G*/LanL2DZ, E= -2382.064596 A.U.

Thermal correction to Gibbs Free Energy= 0.453076 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2383.677939 A.U.

Imaginary frequency -207.1578 cm^{-1}

0 1

C -4.24531 -0.19474 2.86662
C -3.43314 -1.05521 2.13603
C -2.81658 -0.60297 0.95820
C -3.05511 0.70786 0.49264
C -3.81868 1.59846 1.27423
C -4.41467 1.12783 2.45257
N -1.86737 -1.37711 0.24385
Pd 0.11021 -0.63791 0.19767
P 2.21375 0.19722 0.35489
C 3.44254 -0.68911 -0.65070
C 3.31345 -1.84506 -1.37711
C 4.59015 -2.10594 -1.96948
C 5.40459 -1.08614 -1.56790
O 4.72991 -0.21779 -0.76963
C 2.90059 0.15442 2.03762
C 2.53112 1.94141 -0.08859
C 3.29303 -0.06511 4.24354
C 4.43712 0.32469 3.60922
O 4.22218 0.46511 2.27378
O 2.11286 2.33299 -1.34054
C 2.38667 3.66400 -1.46293
C 2.95795 4.13824 -0.32029
C 3.05400 3.02034 0.57227
C 2.29639 -0.17811 3.22234
C -3.98891 3.06156 0.90873
C -4.76279 3.34380 -0.39304
C -3.94976 3.08972 -1.66627
C -3.47791 1.64374 -1.87195
C -2.42578 1.11816 -0.83420
C -1.74291 -0.03334 -1.53212
C -0.60596 0.18914 -2.39562
C -0.35528 -0.60028 -3.47294
C 0.75353 -0.37338 -4.44981
C -1.28463 -3.98992 0.95133
S -2.19276 -2.95105 -0.22128
O -3.62584 -3.25452 -0.06226
O -1.55687 -3.16316 -1.53657
H -4.72702 -0.54825 3.77492
H -3.27225 -2.07238 2.47532
H -5.01211 1.80966 3.05343
H 2.40683 -2.42738 -1.47211
H 4.86205 -2.93468 -2.60911
H 6.43986 -0.84147 -1.75593
H 3.17445 -0.25238 5.30208
H 5.44280 0.53113 3.94551
H 2.12063 4.11232 -2.40867
H 3.27858 5.15440 -0.13419
H 3.46902 3.01485 1.56976
H 1.26056 -0.46687 3.33648
H -3.00016 3.54227 0.83839
H -4.50486 3.55730 1.73944
H -5.07789 4.39644 -0.38868
H -5.68207 2.74169 -0.40818
H -3.07363 3.75636 -1.67233
H -4.55418 3.37319 -2.53917
H -3.02933 1.58087 -2.87198
H -4.33698 0.95979 -1.86798
H -1.68289 1.91191 -0.66362
H -2.41887 -0.79105 -1.91173
H 0.01911 1.05916 -2.20382
H -0.97100 -1.48767 -3.61744
H 1.31226 0.54261 -4.23143
H 0.36862 -0.31374 -5.47773
H 1.46097 -1.21574 -4.43401
H -1.67285 -3.81730 1.95704
H -0.22606 -3.73170 0.89265
H -1.45385 -5.02658 0.64770

CP_{anti}

B3LYP/6-31+G*/LanL2DZ, E= -2382.107825 A.U.

Thermal correction to Gibbs Free Energy= 0.452304 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2383.718659 A.U.

0 1

C -2.90348 -2.51399 -2.33600
C -2.32925 -1.24470 -2.26440
C -2.48283 -0.52615 -1.07860
C -3.18609 -1.04769 0.00883
C -3.72707 -2.34041 -0.04230
C -3.58458 -3.05566 -1.24130
N -1.90485 0.77046 -0.76254
Pd 0.33790 0.28653 -0.37334
P 2.44710 -0.27495 0.05718
C 3.61457 1.11612 0.20712
C 3.41987 2.45859 0.00737
C 4.66614 3.10586 0.28463
C 5.53176 2.11190 0.64089
O 4.91578 0.90162 0.60186
C 3.24666 -1.37816 -1.15182
C 2.76789 -1.19916 1.60232
C 3.77719 -2.75216 -2.85653
C 4.88476 -2.51564 -2.09441
O 4.58599 -1.68913 -1.05717
O 2.28498 -0.62509 2.75442
C 2.56167 -1.47724 3.78093
C 3.20009 -2.58924 3.31736
C 3.33656 -2.40875 1.90160
C 2.71546 -2.01157 -2.24527
C -4.40039 -2.98191 1.15426
C -5.54694 -2.18383 1.80750
C -5.10916 -0.96864 2.64090
C -4.51548 0.20166 1.84449
C -3.16241 -0.08182 1.16778
C -2.56798 1.22154 0.55433
C -1.61452 1.92682 1.47148
C -1.78196 3.17869 1.91353
C -0.86437 3.88051 2.87306
C -0.67710 1.89319 -3.05301
S -2.15560 2.02688 -2.02951
O -3.32825 1.67243 -2.83851
O -2.10552 3.31934 -1.34000
H -2.81256 -3.08961 -3.25333
H -1.79207 -0.84367 -3.11524
H -4.00581 -4.05559 -1.31587
H 2.48744 2.91743 -0.29080
H 4.88496 4.16384 0.23253
H 6.56999 2.09963 0.93932
H 3.72432 -3.37123 -3.74186
H 5.91376 -2.83931 -2.15392
H 2.24655 -1.14880 4.76021
H 3.53840 -3.43104 3.90659
H 3.80636 -3.08210 1.19922
H 1.68344 -1.94899 -2.56081
H -3.63978 -3.18860 1.92460
H -4.78531 -3.96096 0.84378
H -6.09462 -2.86985 2.46803
H -6.25850 -1.86528 1.03235
H -4.38459 -1.29614 3.40262
H -5.98196 -0.59523 3.19373
H -4.37570 1.05350 2.52457
H -5.23382 0.52535 1.07742
H -2.46393 -0.45542 1.93367
H -3.39641 1.89072 0.29763
H -0.75741 1.33531 1.80193
H -2.62874 3.75816 1.54275
H -0.03006 3.23932 3.17747
H -1.40244 4.19808 3.77711
H -0.44972 4.79073 2.41821
H -0.69859 0.95769 -3.61167
H 0.20191 1.94182 -2.40454
H -0.72928 2.74841 -3.73315

INT3

B3LYP/6-31+G*/LanL2DZ, E= -2393.608816 A.U.

Thermal correction to Gibbs Free Energy= 0.449224 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.257525 A.U.

-1 1

C -5.60045 2.11989 0.79651
C -5.34179 0.75533 0.82796
C -4.20162 0.21750 0.17195
C -3.28433 1.12667 -0.43701
C -3.60287 2.49678 -0.52680
C -4.75783 2.99067 0.09707
N -3.94602 -1.12973 0.00058
Pd 0.92241 -1.11528 -0.26701
P 1.86434 0.96373 0.41392
I 3.28596 -2.58370 -0.57294
C 2.82613 1.81468 -0.87157
C 3.20755 1.35148 -2.10261
C 4.01093 2.37505 -2.69982
C 4.06736 3.38969 -1.78911
O 3.35998 3.07197 -0.67135
C 3.00296 0.85945 1.83463
C 0.74117 2.27947 0.99616
C 4.35193 0.31452 3.54787
C 4.23344 1.67230 3.47223
O 3.42047 2.02603 2.44299
O -0.29425 1.83033 1.78284
C -1.00989 2.91459 2.17930
C -0.46208 4.05598 1.67034
C 0.67638 3.64553 0.90339
C 3.55099 -0.21381 2.48531
C -2.76412 3.45187 -1.35611
C -2.73315 3.09565 -2.86003
C -1.75902 1.96767 -3.23547
C -1.98633 0.59093 -2.58389
C -1.95686 0.62822 -1.03334
C -1.44504 -0.64246 -0.36544
C -1.07304 -1.81987 -1.03442
C -0.42793 -2.88262 -0.37671
C -0.08243 -4.16934 -1.07604
C -4.32507 -3.71658 -0.03425
S -4.37687 -2.26890 1.05135
O -3.33437 -2.50745 2.09505
O -5.77548 -2.19531 1.57316
H -6.48752 2.50730 1.29638
H -6.02338 0.07253 1.32193
H -4.99406 4.05137 0.02917
H 2.96242 0.37814 -2.50477
H 4.48524 2.35334 -3.67172
H 4.54366 4.35944 -1.78083
H 4.93316 -0.24438 4.26908
H 4.63834 2.49045 4.05027
H -1.88451 2.70443 2.77630
H -0.83316 5.06271 1.80805
H 1.36969 4.27493 0.36529
H 3.41306 -1.24961 2.20901
H -1.73168 3.50978 -0.98181
H -3.18269 4.46035 -1.24183
H -2.44002 3.99187 -3.42802
H -3.75155 2.83835 -3.18461
H -0.73878 2.29726 -2.98330
H -1.77390 1.83997 -4.32827
H -1.18480 -0.05749 -2.95899
H -2.93644 0.15321 -2.91751
H -1.21505 1.39240 -0.76391
H -1.54046 -0.67934 0.71510
H -1.16627 -1.87646 -2.11620
H -0.54990 -2.94960 0.70642
H 0.07882 -4.01730 -2.14902
H -0.90399 -4.89187 -0.94876
H 0.82542 -4.61514 -0.66068
H -3.33064 -3.79167 -0.47795
H -5.08642 -3.60351 -0.80883
H -4.53528 -4.58792 0.59171

TS_B

B3LYP/6-31+G*/LanL2DZ, E= -2393.607721 A.U.

Thermal correction to Gibbs Free Energy= 0.449268 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.255848 A.U.

Imaginary frequency -94.6192 cm^{-1}

-1 1

C -6.08506 1.77881 0.84766
C -5.67732 0.44863 0.79883
C -4.42625 0.11614 0.22765
C -3.58770 1.16016 -0.24142
C -4.03674 2.49112 -0.24477
C -5.28765 2.79568 0.31407
N -3.93708 -1.16232 -0.01243
Pd 0.94775 -1.10175 -0.25492
P 1.98366 0.97401 0.30795
I 3.25551 -2.71014 -0.40399
C 2.99564 1.68375 -1.02785
C 3.33434 1.12011 -2.22921
C 4.20948 2.04149 -2.88876
C 4.34781 3.10215 -2.04107
O 3.62458 2.90749 -0.90566
C 3.11692 0.92368 1.73884
C 0.97291 2.42078 0.80021
C 4.44219 0.43164 3.48668
C 4.38923 1.78543 3.31960
O 3.59207 2.10780 2.26774
O 0.04195 2.15249 1.77733
C -0.59030 3.31924 2.07605
C -0.09815 4.33369 1.30868
C 0.91789 3.75200 0.48054
C 3.61382 -0.12792 2.46155
C -3.23131 3.59254 -0.90434
C -3.04641 3.39177 -2.42510
C -1.96082 2.37437 -2.81039
C -2.14742 0.92105 -2.33629
C -2.21774 0.76784 -0.79564
C -1.78130 -0.59114 -0.25687
C -1.13760 -1.58681 -1.01996
C -0.47320 -2.71614 -0.47785
C -0.15360 -3.91791 -1.33413
C -4.12164 -3.77522 -0.29227
S -4.26614 -2.44967 0.92691
O -3.19729 -2.69211 1.93259
O -5.66327 -2.50031 1.43915
H -7.05010 2.02316 1.28912
H -6.31088 -0.34336 1.17844
H -5.63396 3.82777 0.32329
H 3.01469 0.14461 -2.56894
H 4.67685 1.92444 -3.85730
H 4.89764 4.03097 -2.09169
H 4.99844 -0.10484 4.24384
H 4.83477 2.62010 3.84156
H -1.36856 3.25222 2.82150
H -0.42144 5.36612 1.32388
H 1.54675 4.25566 -0.23852
H 3.42566 -1.17200 2.25405
H -2.24113 3.69119 -0.43759
H -3.74674 4.54672 -0.73220
H -2.77371 4.35828 -2.87547
H -4.01053 3.10161 -2.86718
H -0.99577 2.73674 -2.42407
H -1.86374 2.36570 -3.90623
H -1.28593 0.36320 -2.72048
H -3.04637 0.47888 -2.78707
H -1.48676 1.47499 -0.37659
H -1.73725 -0.67810 0.82347
H -1.20460 -1.52923 -2.10388
H -0.63977 -2.92970 0.58053
H 0.06321 -3.62936 -2.36924
H -1.00768 -4.61466 -1.34727
H 0.71547 -4.45795 -0.95003
H -3.13799 -3.71852 -0.76029
H -4.91228 -3.65261 -1.03515
H -4.23844 -4.71812 0.24862

CP_{syn}

B3LYP/6-31+G*/LanL2DZ, E= -2393.624616 A.U.

Thermal correction to Gibbs Free Energy= 0.45348 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.271588 A.U.

-1 1

C -6.65278 1.18046 0.29180
C -5.97839 -0.04373 0.28521
C -4.58452 -0.02749 0.14185
C -3.89387 1.18007 -0.02495
C -4.57617 2.40115 -0.05085
C -5.96841 2.38779 0.12969
N -3.67876 -1.12452 0.03921
Pd 0.87961 -0.99638 -0.35163
P 2.02296 0.98872 0.15134
I 3.14819 -2.83431 -0.22435
C 3.32555 1.40744 -1.06113
C 3.72757 0.69244 -2.15770
C 4.83785 1.39314 -2.72900
C 5.04186 2.48592 -1.93670
O 4.14063 2.51562 -0.91882
C 2.93519 0.92357 1.73930
C 1.29117 2.66759 0.38088
C 3.96167 0.39998 3.67032
C 4.07040 1.74214 3.44496
O 3.45723 2.08301 2.28103
O 0.35693 2.76382 1.38762
C -0.05850 4.06013 1.44628
C 0.57117 4.80098 0.49034
C 1.44622 3.89878 -0.20111
C 3.22239 -0.13056 2.56448
C -3.84374 3.69277 -0.33843
C -3.23125 3.73752 -1.75551
C -1.95287 2.90115 -1.93292
C -2.05322 1.37733 -1.73709
C -2.42659 0.93930 -0.29929
C -2.21951 -0.58342 0.03353
C -1.30079 -1.33056 -0.89992
C -0.62810 -2.53425 -0.62886
C -0.28700 -3.52022 -1.72976
C -3.87884 -3.79849 -0.45792
S -3.96181 -2.58588 0.87036
O -2.86183 -2.84979 1.80749
O -5.34677 -2.60869 1.37135
H -7.73314 1.18562 0.42065
H -6.51785 -0.97140 0.41354
H -6.51733 3.32774 0.12633
H 3.29868 -0.24846 -2.47321
H 5.41308 1.11195 -3.60120
H 5.75289 3.29965 -1.95612
H 4.35712 -0.14727 4.51599
H 4.52595 2.55661 3.98997
H -0.79064 4.28418 2.20792
H 0.43553 5.85827 0.30232
H 2.12822 4.13647 -1.00382
H 2.96078 -1.16140 2.36953
H -3.03953 3.85113 0.39526
H -4.54463 4.52968 -0.21957
H -2.98413 4.78307 -1.99243
H -3.99452 3.42421 -2.48317
H -1.18569 3.28845 -1.24994
H -1.56677 3.08087 -2.94716
H -1.06979 0.96020 -1.97523
H -2.77264 0.95225 -2.45283
H -1.78986 1.50968 0.38739
H -1.86611 -0.67963 1.06251
H -1.46532 -1.11404 -1.95568
H -0.69289 -2.95723 0.37410
H -0.18699 -3.01509 -2.69851
H -1.07035 -4.29191 -1.83989
H 0.65517 -4.03434 -1.52008
H -2.90737 -3.72389 -0.94390
H -4.68885 -3.58674 -1.15869
H -4.01116 -4.77939 0.00681

SM$_{ZE}$

B3LYP/6-31+G*/LanL2DZ, E= -1237.1045 A.U.

Thermal correction to Gibbs Free Energy= 0.284073 A.U.

SP at B3LYP/6-311++G**/SDD, E= -1237.37472 A.U.

-1 1

C -0.47832 -1.60622 2.81176

C -1.40334 -0.87008 2.07983

C -1.21961 -0.61316 0.69034

C -0.01871 -1.15223 0.12245

C 0.93343 -1.87530 0.85012

C 0.67697 -2.10939 2.21636

N -2.06138 0.09243 -0.12859

I 0.24199 -0.79113 -1.99546

C 2.21030 -2.46971 0.27285

C 3.53724 -1.95358 0.87903

C 4.01289 -0.55561 0.44187

C 3.17816 0.63786 0.95020

C 3.90552 1.94448 0.77089

C 3.42408 3.12645 0.32974

C 2.05937 3.49296 -0.06996

C 0.89754 3.03668 0.43663

C -0.46531 3.43428 -0.04493

C -4.54345 -0.98617 0.30726

S -3.54428 0.54292 0.30925

O -3.67794 1.09036 1.69314

O -4.10030 1.38153 -0.77720

H -0.66142 -1.78257 3.87112

H -2.27043 -0.44072 2.56863

H 1.39014 -2.68850 2.79974

H 2.24196 -2.33622 -0.81144

H 2.17431 -3.55600 0.44592

H 4.32181 -2.67167 0.59491

H 3.47922 -1.98590 1.97665

H 4.06491 -0.51248 -0.65564

H 5.04741 -0.43223 0.80085

H 2.95600 0.48190 2.01879

H 2.20965 0.66694 0.44362

H 4.97139 1.91247 1.01293

H 4.15489 3.93142 0.21752

H 2.00217 4.24849 -0.85852

H 0.91794 2.32387 1.26038

H -1.02214 2.55668 -0.39991

H -0.40785 4.16809 -0.85853

H -1.06501 3.86192 0.77066

H -4.52849 -1.40024 -0.70332

H -5.56162 -0.71638 0.60105

H -4.11672 -1.69539 1.02209

CP1'

B3LYP/6-31+G*/LanL2DZ, E= -2393.564836 A.U.

Thermal correction to Gibbs Free Energy= 0.446311 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.215942 A.U.

-1 1

C -5.03017 -0.67564 -0.69163
C -4.24913 0.44687 -0.97782
C -2.89496 0.49630 -0.56641
C -2.37788 -0.63563 0.11793
C -3.17916 -1.70218 0.50960
C -4.51791 -1.73053 0.06060
N -1.98995 1.54482 -0.71230
Pd -0.36213 -0.41557 0.34093
P 2.12802 0.01992 0.20397
I -0.18490 -2.10802 -1.83684
C 3.03042 0.04684 1.80492
C 3.99089 0.83687 2.38061
C 4.21025 0.32707 3.70204
C 3.37058 -0.73966 3.84016
O 2.64415 -0.92102 2.70583
C 2.54067 1.64353 -0.47877
C 3.22357 -1.06506 -0.77548
C 2.57234 3.71344 -1.34659
C 3.85217 3.28948 -1.14101
O 3.86627 2.03382 -0.61365
O 3.43288 -2.32235 -0.27127
C 4.19020 -3.00018 -1.17613
C 4.47540 -2.20592 -2.24730
C 3.84680 -0.94445 -1.98711
C 1.71782 2.64626 -0.91673
C -2.74707 -2.75473 1.51517
C -3.48518 -2.56495 2.86870
C -3.05081 -1.39332 3.78755
C -2.57106 -0.07720 3.13618
C -1.11369 -0.14093 2.71658
C -0.31303 0.94714 2.43916
C -0.73404 2.33587 2.30213
C 0.12924 3.34715 2.51493
C -0.19359 4.80651 2.40790
C -2.20115 2.16142 -3.37751
S -2.29105 2.79341 -1.66858
O -3.64798 3.40312 -1.54582
O -1.14781 3.74003 -1.53198
H -6.06453 -0.70591 -1.03397
H -4.68458 1.30095 -1.48591
H -5.15519 -2.57411 0.32749
H 4.48313 1.67383 1.90691
H 4.89871 0.70554 4.44611
H 3.17279 -1.43759 4.64024
H 2.25364 4.66160 -1.75761
H 4.82327 3.73198 -1.31264
H 4.43050 -4.01966 -0.91406
H 5.05075 -2.48342 -3.12051
H 3.84294 -0.06878 -2.61998
H 0.63265 2.65495 -0.94226
H -1.65956 -2.74223 1.64396
H -3.00231 -3.75487 1.13532
H -3.39720 -3.49243 3.45533
H -4.55217 -2.45266 2.64006
H -2.24509 -1.74043 4.45375
H -3.89769 -1.16310 4.44978
H -2.63847 0.71751 3.88989
H -3.22632 0.22542 2.31620
H -0.58646 -1.05929 2.97688
H 0.75702 0.80768 2.56208
H -1.76085 2.54164 2.00875
H 1.16295 3.10048 2.76893
H -1.23606 4.96667 2.11356
H 0.44236 5.28971 1.65244
H -0.01254 5.32842 3.36004
H -1.19921 1.75876 -3.54007
H -2.40575 2.99344 -4.05743
H -2.94823 1.37312 -3.50124

TS_{Heck}'

B3LYP/6-31+G*/LanL2DZ, E= -2393.528508 A.U.

Thermal correction to Gibbs Free Energy= 0.446298 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.178859 A.U.

Imaginary frequency -329.2065 cm^{-1}

-1 1

C -4.92478 -0.82181 -0.80602
C -4.17446 0.33408 -0.99287
C -2.86087 0.44205 -0.46375
C -2.37066 -0.65326 0.32477
C -3.16167 -1.78785 0.55859
C -4.42712 -1.88011 -0.04478
N -1.98483 1.49180 -0.66836
Pd -0.22088 -0.44182 0.21213
P 2.12613 -0.05030 0.10110
I -0.17352 -2.21086 -1.94479
C 3.00731 -0.02952 1.71514
C 3.97699 0.75493 2.28332
C 4.21031 0.23825 3.59962
C 3.36874 -0.82636 3.74209
O 2.62837 -0.99992 2.61498
C 2.55732 1.56995 -0.57476
C 3.22391 -1.14571 -0.86289
C 2.60307 3.64370 -1.43032
C 3.87991 3.20958 -1.22662
O 3.88481 1.95115 -0.70596
O 3.43612 -2.39942 -0.35175
C 4.19897 -3.07835 -1.25081
C 4.48656 -2.28771 -2.32413
C 3.85243 -1.02781 -2.07205
C 1.74145 2.58064 -1.00613
C -2.82273 -2.86091 1.57804
C -3.57437 -2.59927 2.91150
C -3.14626 -1.37426 3.75663
C -2.80312 -0.06963 3.00268
C -1.47668 -0.25130 2.25563
C -0.46539 0.74586 2.13109
C -0.73785 2.17822 2.08435
C 0.15146 3.11869 2.46206
C -0.09454 4.59858 2.40403
C -2.17174 1.97363 -3.36871
S -2.29201 2.69066 -1.69730
O -3.65465 3.29389 -1.61813
O -1.15761 3.64943 -1.59592
H -5.91610 -0.89241 -1.25189
H -4.58775 1.16872 -1.54797
H -5.03049 -2.77257 0.11581
H 4.46740 1.59187 1.80787
H 4.90839 0.61135 4.33743
H 3.17681 -1.52719 4.54108
H 2.29262 4.59731 -1.83505
H 4.85411 3.64613 -1.39575
H 4.44034 -4.09637 -0.98414
H 5.06554 -2.56735 -3.19421
H 3.84701 -0.15533 -2.70927
H 0.65697 2.59635 -1.02569
H -1.74278 -2.95627 1.72784
H -3.16069 -3.83295 1.19395
H -3.49236 -3.49166 3.55122
H -4.63881 -2.49739 2.66220
H -2.26424 -1.64440 4.35773
H -3.94721 -1.16638 4.48120
H -2.65289 0.72876 3.74558
H -3.62436 0.25209 2.35740
H -1.03575 -1.21337 2.50283
H 0.50739 0.46688 2.53141
H -1.70521 2.48517 1.69513
H 1.13850 2.80173 2.80759
H -1.09861 4.82051 2.02734
H 0.62616 5.09026 1.73427
H 0.01944 5.06870 3.39301
H -1.16759 1.56380 -3.49402
H -2.36251 2.77725 -4.08535
H -2.91586 1.18038 -3.47310

INT1’

B3LYP/6-31+G*/LanL2DZ, E= -2393.606087 A.U.

Thermal correction to Gibbs Free Energy= 0.451738 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.256218 A.U.

-1 1

C -4.85457 -0.80925 -0.86681
C -4.15834 0.38453 -0.93724
C -2.93329 0.57115 -0.23568
C -2.57420 -0.43355 0.75198
C -3.28254 -1.66553 0.75480
C -4.38552 -1.86214 -0.07405
N -2.06005 1.60477 -0.47517
Pd -0.12516 -0.30938 0.22109
P 2.11285 0.05206 0.21079
I -0.18885 -2.14014 -1.88393
C 2.98425 0.06449 1.82135
C 3.95917 0.84573 2.38422
C 4.19969 0.32241 3.69605
C 3.35686 -0.74163 3.83854
O 2.60945 -0.90914 2.71588
C 2.54604 1.66554 -0.47803
C 3.19407 -1.05369 -0.76070
C 2.60164 3.73271 -1.34693
C 3.87641 3.29188 -1.14425
O 3.87477 2.03686 -0.61585
O 3.41061 -2.30817 -0.25399
C 4.17309 -2.98233 -1.15654
C 4.45745 -2.18769 -2.22813
C 3.82033 -0.93093 -1.97140
C 1.73521 2.67819 -0.91320
C -2.99670 -2.75034 1.77869
C -3.68007 -2.44871 3.13465
C -3.10567 -1.28271 3.97276
C -2.82978 0.04888 3.24126
C -1.79181 -0.17546 2.09075
C -0.58114 0.75018 2.03477
C -0.74313 2.20844 2.02764
C 0.12267 3.09040 2.56889
C -0.06374 4.58241 2.52408
C -2.16522 1.98629 -3.21929
S -2.32531 2.76073 -1.57804
O -3.68356 3.37322 -1.54563
O -1.18393 3.70962 -1.48727
H -5.76558 -0.93220 -1.45301
H -4.53397 1.19646 -1.54822
H -4.91012 -2.81627 -0.05911
H 4.44715 1.68415 1.90899
H 4.90230 0.69124 4.43169
H 3.16837 -1.44534 4.63579
H 2.29678 4.68640 -1.75570
H 4.85282 3.72128 -1.31862
H 4.41700 -4.00070 -0.89356
H 5.03533 -2.46344 -3.10014
H 3.81093 -0.05716 -2.60674
H 0.65161 2.70058 -0.92642
H -1.92202 -2.92514 1.90799
H -3.40808 -3.69298 1.39655
H -3.64656 -3.35500 3.75882
H -4.74195 -2.25446 2.92779
H -2.15361 -1.61153 4.41954
H -3.78775 -1.10325 4.81819
H -2.43182 0.77182 3.96736
H -3.75138 0.47832 2.82980
H -1.33236 -1.13452 2.34291
H 0.18962 0.43031 2.73945
H -1.62134 2.59647 1.52122
H 1.03809 2.72464 3.04179
H -1.00345 4.84868 2.02646
H 0.75452 5.06831 1.96894
H -0.06575 5.02472 3.53308
H -1.16712 1.55143 -3.29930
H -2.31135 2.77842 -3.95861
H -2.92263 1.20803 -3.33250

INT2’

B3LYP/6-31+G*/LanL2DZ, E= -2382.091835 A.U.

Thermal correction to Gibbs Free Energy= 0.457076 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2383.70797 A.U.

0 1

C 5.07432 -0.36932 2.10155
C 4.01398 -1.14431 1.64972
C 3.10648 -0.63290 0.70188
C 3.25710 0.69017 0.19719
C 4.33111 1.47300 0.68853
C 5.22485 0.93329 1.62529
N 2.00919 -1.43839 0.31435
Pd 0.17916 -0.59294 0.06581
P -2.10946 0.07272 0.32508
C -3.21166 -0.80946 -0.80749
C -2.95510 -1.88462 -1.61904
C -4.18982 -2.20965 -2.26540
C -5.10570 -1.30697 -1.80597
O -4.53479 -0.45072 -0.91813
C -2.65113 1.80344 0.20749
C -2.72928 -0.36079 1.98306
C -3.32198 3.93862 0.39559
C -2.81477 3.72667 -0.85191
O -2.39589 2.43728 -0.98319
O -4.07181 -0.21771 2.26271
C -4.26797 -0.65031 3.53684
C -3.09332 -1.07068 4.08941
C -2.09442 -0.88494 3.07998
C -3.21808 2.68761 1.08642
C 4.55284 2.91236 0.25587
C 3.44952 3.89550 0.70130
C 2.17294 3.83343 -0.14765
C 1.45155 2.47682 -0.16664
C 2.26030 1.31238 -0.80630
C 1.39330 0.26180 -1.49611
C 0.44149 0.45503 -2.59283
C -0.00829 1.56413 -3.21301
C -0.95898 1.50986 -4.37426
C 3.74130 -2.87495 -1.37142
S 2.21573 -2.93177 -0.38615
O 2.43475 -3.96574 0.64286
O 1.09394 -3.11516 -1.33372
H 5.76802 -0.76994 2.83679
H 3.84695 -2.14648 2.03299
H 6.04422 1.54944 1.98847
H -1.99805 -2.37879 -1.72944
H -4.36760 -3.00362 -2.97783
H -6.15440 -1.14215 -2.00587
H -3.72668 4.86589 0.77785
H -2.68803 4.35166 -1.72334
H -5.28516 -0.59788 3.89669
H -2.95274 -1.46723 5.08553
H -1.03937 -1.11413 3.15351
H -3.53347 2.47036 2.09653
H 4.66193 2.97553 -0.83803
H 5.51048 3.24594 0.67223
H 3.85098 4.91711 0.64852
H 3.20702 3.70922 1.75704
H 2.42331 4.11947 -1.18196
H 1.46895 4.59498 0.21580
H 0.51029 2.59562 -0.71198
H 1.17367 2.18782 0.85514
H 2.86884 1.74752 -1.62161
H 0.09959 -0.49908 -2.99758
H 0.30923 2.55321 -2.88644
H -0.56005 2.03818 -5.25150
H -1.91345 1.99352 -4.12007
H -1.17398 0.47598 -4.66557
H 4.58797 -2.63231 -0.72727
H 3.63285 -2.13764 -2.17110
H 3.85604 -3.87848 -1.79038
H 2.00647 -0.58973 -1.77021

TS_A'

B3LYP/6-31+G*/LanL2DZ, E= -2382.050758 A.U.

Thermal correction to Gibbs Free Energy= 0.454719 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2383.664427 A.U.

Imaginary frequency -226.8964 cm^{-1}

0 1

C 4.95339 -0.44326 2.14901
C 3.91094 -1.18827 1.59992
C 3.11300 -0.61654 0.59275
C 3.36533 0.70219 0.15743
C 4.38403 1.46527 0.75128
C 5.18535 0.87182 1.73670
N 2.01934 -1.28294 -0.01461
Pd 0.02475 -0.62760 0.14730
P -2.15100 -0.01995 0.41092
C -3.25583 -0.87717 -0.74928
C -3.00047 -1.94589 -1.56964
C -4.22786 -2.25075 -2.24038
C -5.14072 -1.34240 -1.78623
O -4.57348 -0.50189 -0.88096
C -2.68588 1.72008 0.25743
C -2.81982 -0.42708 2.05143
C -3.34820 3.86450 0.41184
C -2.83039 3.63621 -0.82791
O -2.41510 2.34164 -0.93956
O -4.15945 -0.26790 2.33389
C -4.35584 -0.69742 3.60912
C -3.18342 -1.12880 4.15913
C -2.18685 -0.95585 3.14632
C -3.25645 2.62005 1.11763
C 4.58392 2.92140 0.37874
C 3.39724 3.83238 0.77264
C 2.15264 3.73222 -0.12767
C 1.48853 2.34695 -0.23160
C 2.41777 1.28780 -0.88045
C 1.78481 0.14155 -1.63440
C 0.65420 0.19411 -2.56124
C 0.11617 1.29201 -3.13729
C -0.94431 1.23920 -4.19627
C 3.72710 -3.00453 -1.41598
S 2.16522 -2.88523 -0.49955
O 2.31041 -3.76602 0.67167
O 1.07256 -3.12512 -1.45731
H 5.57547 -0.88630 2.92295
H 3.69616 -2.19273 1.94824
H 5.98594 1.44957 2.19300
H -2.04704 -2.44898 -1.66628
H -4.40406 -3.03579 -2.96329
H -6.18448 -1.16405 -2.00030
H -3.75379 4.79769 0.77893
H -2.69487 4.24989 -1.70615
H -5.37140 -0.63565 3.97236
H -3.04583 -1.52551 5.15577
H -1.13435 -1.19749 3.20523
H -3.58471 2.41550 2.12637
H 4.77123 3.02308 -0.70159
H 5.48920 3.28622 0.87853
H 3.74356 4.87503 0.75405
H 3.11796 3.61630 1.81330
H 2.42161 4.07348 -1.14050
H 1.40387 4.44573 0.24200
H 0.56181 2.44502 -0.80128
H 1.19284 1.98937 0.76233
H 3.02826 1.80280 -1.64606
H 0.34307 -0.78445 -2.92464
H 0.44946 2.28502 -2.84463
H -0.63722 1.78272 -5.10064
H -1.86857 1.71380 -3.83633
H -1.18396 0.20849 -4.47838
H 4.55216 -2.68442 -0.77724
H 3.66851 -2.39724 -2.32186
H 3.83694 -4.05957 -1.67773
H 2.55011 -0.51884 -2.03105

CP_{anti}'

B3LYP/6-31+G*/LanL2DZ, E= -2382.104924 A.U.

Thermal correction to Gibbs Free Energy= 0.452251 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2383.71557 A.U.

0 1

C 4.90222 -0.39565 2.13610
C 3.87784 -1.11372 1.50725
C 3.20439 -0.48603 0.45418
C 3.52087 0.82167 0.08342
C 4.49005 1.56539 0.75589
C 5.20814 0.92066 1.77297
N 2.11971 -0.99045 -0.38681
Pd -0.02712 -0.56851 0.19256
P -2.14471 0.01606 0.42215
C -3.24281 -0.83020 -0.75529
C -2.98261 -1.89550 -1.57889
C -4.20220 -2.19359 -2.26629
C -5.11713 -1.28387 -1.81887
O -4.55734 -0.44976 -0.90353
C -2.66414 1.76207 0.24768
C -2.83132 -0.37780 2.05305
C -3.30861 3.91452 0.38851
C -2.78788 3.67573 -0.84814
O -2.38270 2.37689 -0.95108
O -4.16726 -0.21543 2.34589
C -4.35355 -0.64445 3.62242
C -3.17694 -1.07734 4.16338
C -2.18945 -0.90688 3.14255
C -3.22986 2.67251 1.10048
C 4.66834 3.03025 0.42361
C 3.41725 3.87721 0.76665
C 2.20106 3.72192 -0.17068
C 1.57961 2.31610 -0.31786
C 2.58105 1.32451 -0.97477
C 2.09578 -0.02165 -1.59786
C 0.82334 0.00025 -2.41585
C 0.41080 1.07802 -3.10550
C -0.77412 1.12319 -4.02880
C 3.78021 -2.99199 -1.51836
S 2.19151 -2.72998 -0.69155
O 2.25350 -3.39751 0.61047
O 1.12069 -3.05171 -1.63556
H 5.45487 -0.87096 2.94251
H 3.62139 -2.11313 1.83245
H 5.99242 1.45784 2.30171
H -2.02988 -2.40027 -1.66573
H -4.37286 -2.97391 -2.99575
H -6.15747 -1.10048 -2.04525
H -3.70847 4.85285 0.74912
H -2.64380 4.28337 -1.72926
H -5.36592 -0.58176 3.99455
H -3.03337 -1.47339 5.15958
H -1.13684 -1.14954 3.18596
H -3.56535 2.47499 2.10833
H 4.90786 3.15539 -0.64342
H 5.52752 3.42288 0.98114
H 3.71082 4.93606 0.75560
H 3.11587 3.65058 1.79895
H 2.48211 4.08599 -1.17233
H 1.41691 4.40303 0.18632
H 0.66650 2.40103 -0.91037
H 1.26732 1.92718 0.65912
H 3.11681 1.86472 -1.76643
H 0.32444 -0.95603 -2.55922
H 0.94464 2.02166 -2.99889
H -0.50169 1.55904 -4.99963
H -1.57203 1.74628 -3.60765
H -1.18866 0.12715 -4.20505
H 4.58380 -2.62861 -0.87544
H 3.77583 -2.48304 -2.48393
H 3.86197 -4.07238 -1.66158
H 2.92555 -0.34805 -2.24830

INT3’

B3LYP/6-31+G*/LanL2DZ, E= -2393.635378 A.U.

Thermal correction to Gibbs Free Energy= 0.450666 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.282423 A.U.

-1 1

C -6.36546 1.94383 1.09188
C -5.97149 0.66139 0.71456
C -4.65517 0.43594 0.24497
C -3.74202 1.52493 0.22979
C -4.16262 2.81867 0.56650
C -5.48265 3.02339 1.00392
N -4.12525 -0.73926 -0.24292
C -3.24794 4.01173 0.37114
C -2.88686 4.26334 -1.11207
C -1.79228 3.34412 -1.68214
C -2.06124 1.82969 -1.66212
C -2.30918 1.25263 -0.24162
C -1.92667 -0.21532 -0.17494
C -1.42299 -0.84511 0.97400
C -0.90328 -2.17081 0.91354
C -0.69975 -2.99090 2.16251
C -5.95489 -1.97308 -1.85941
S -4.90203 -2.14465 -0.38096
O -5.84008 -2.44336 0.73329
O -3.89501 -3.17214 -0.72397
H -7.38025 2.10291 1.45359
H -6.65639 -0.17477 0.80053
H -5.81090 4.02621 1.27109
H -2.31715 3.89981 0.94730
H -3.75023 4.90284 0.76971
H -2.53581 5.30113 -1.21577
H -3.80267 4.18130 -1.71503
H -0.86147 3.53285 -1.12931
H -1.59203 3.64499 -2.72137
H -1.18208 1.33542 -2.09796
H -2.91828 1.57732 -2.30137
H -1.63085 1.77209 0.44931
H -1.14308 -2.74747 0.02107
H -1.63903 -3.50437 2.42163
H -0.40719 -2.36805 3.01660
H 0.07117 -3.75165 2.00843
H -6.64432 -1.13738 -1.71172
H -6.50896 -2.90802 -1.98023
H -5.30839 -1.79401 -2.72128
H -1.52769 -0.34179 1.93482
H -1.84134 -0.75425 -1.11165
H 0.07236 4.25421 2.74836
H 6.19787 -0.22723 2.93803
H 6.29054 2.42115 2.16959
C 5.49565 0.32005 2.32317
C 5.58002 1.63391 1.96208
C 0.64663 4.03933 1.85938
O 0.93306 2.72725 1.64457
C 4.29425 -0.18022 1.72552
O 4.52327 1.98578 1.18337
C 1.15988 4.80814 0.85617
H 1.07743 5.88300 0.76217
H 3.89958 -1.18665 1.76145
C 3.73249 0.86287 1.03818
C 1.66007 2.64532 0.47758
C 1.82034 3.90450 -0.03891
P 2.20535 0.94995 0.03943
Pd 0.73145 -0.90279 0.33439
H 2.36466 4.15096 -0.93826
I 2.45259 -3.04481 -0.24602
C 2.81552 1.19354 -1.65796
O 3.62655 2.25542 -2.01089
C 3.95788 2.08880 -3.32034
C 2.65405 0.36949 -2.73989
H 4.59234 2.85443 -3.74324
H 2.10069 -0.55975 -2.73640
C 3.39241 0.95182 -3.81970
H 3.49260 0.56980 -4.82676

$TS_{B'}$

B3LYP/6-31+G*/LanL2DZ, E= -2393.610569 A.U.

Thermal correction to Gibbs Free Energy= 0.448472 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.25832 A.U.

Imaginary frequency -87.6721 cm^{-1}

-1 1

C -6.23568 1.79847 1.09853
C -5.84033 0.51528 0.72393
C -4.52372 0.29250 0.25596
C -3.61325 1.38233 0.23594
C -4.03394 2.67580 0.57139
C -5.35414 2.87892 1.00923
N -3.98645 -0.88262 -0.22651
C -3.11849 3.86788 0.37530
C -2.75483 4.11667 -1.10772
C -1.66091 3.19491 -1.67513
C -1.93324 1.68096 -1.65690
C -2.18398 1.10294 -0.23767
C -1.81697 -0.37014 -0.17318
C -1.29456 -0.99378 0.97377
C -0.77331 -2.31822 0.91676
C -0.56824 -3.13548 2.16764
C -5.81330 -2.11155 -1.85170
S -4.76308 -2.28940 -0.37237
O -5.70315 -2.58937 0.73916
O -3.75495 -3.31463 -0.71653
H -7.25061 1.95703 1.45995
H -6.52397 -0.32166 0.81205
H -5.68366 3.88147 1.27581
H -2.18866 3.75537 0.95288
H -3.62036 4.76010 0.77194
H -2.40177 5.15367 -1.21210
H -3.66986 4.03560 -1.71205
H -0.73104 3.38129 -1.12000
H -1.45739 3.49575 -2.71371
H -1.05454 1.18507 -2.09171
H -2.78997 1.43137 -2.29782
H -1.49962 1.61440 0.45312
H -1.01024 -2.89751 0.02525
H -1.50588 -3.65181 2.42717
H -0.27873 -2.50989 3.02077
H 0.20567 -3.89369 2.01589
H -6.50182 -1.27540 -1.70272
H -6.36837 -3.04551 -1.97525
H -5.16541 -1.93140 -2.71227
H -1.39946 -0.48910 1.93392
H -1.72354 -0.90520 -1.11131
H 0.20418 4.10925 2.75531
H 6.32983 -0.37415 2.94344
H 6.42179 2.27442 2.17557
C 5.62713 0.17322 2.32920
C 5.71119 1.48717 1.96834
C 0.77803 3.89382 1.86619
O 1.06433 2.58163 1.65199
C 4.42536 -0.32701 1.73220
O 4.65389 1.83912 1.19038
C 1.29121 4.66206 0.86248
H 1.20903 5.73692 0.76803
H 4.03075 -1.33349 1.76795
C 3.86301 0.71616 1.04549
C 1.79130 2.49887 0.48501
C 1.95151 3.75782 -0.03217
P 2.33492 0.80236 0.04759
Pd 0.86296 -1.05009 0.34177
H 2.49593 4.00374 -0.93160
I 2.58544 -3.19280 -0.24054
C 2.94583 1.04635 -1.64998
O 3.75675 2.10845 -2.00293
C 4.08866 1.94170 -3.31223
C 2.78512 0.22210 -2.73187
H 4.72312 2.70741 -3.73501
H 2.23230 -0.70747 -2.72816
C 3.52373 0.80444 -3.81156
H 3.62455 0.42217 -4.81848

CP_{syn}'

B3LYP/6-31+G*/LanL2DZ, E= -2393.635378 A.U.

Thermal correction to Gibbs Free Energy= 0.450664 A.U.

SP at B3LYP/6-311++G**/SDD, E= -2395.282422 A.U.

-1 1

C -6.36527 1.94290 1.12981
C -5.92050 0.64348 0.85807
C -4.60687 0.49029 0.39806
C -3.76429 1.59610 0.22335
C -4.20776 2.88914 0.50354
C -5.52767 3.04968 0.96126
N -3.91241 -0.69151 0.05663
C -3.29744 4.07463 0.27086
C -2.85254 4.23902 -1.20086
C -1.76961 3.25708 -1.68911
C -2.12312 1.75791 -1.70815
C -2.41680 1.17422 -0.31114
C -2.42818 -0.38852 -0.23973
C -1.52632 -0.91696 0.84966
C -0.98199 -2.20545 0.84719
C -0.69157 -2.96325 2.12464
C -5.66158 -1.70304 -1.84749
S -4.70404 -2.10247 -0.35759
O -5.69201 -2.41322 0.68807
O -3.69417 -3.09004 -0.74472
H -7.38078 2.08742 1.49242
H -6.55861 -0.21545 1.02914
H -5.89772 4.04814 1.18657
H -2.39919 3.98996 0.90067
H -3.81717 4.98742 0.59097
H -2.45319 5.25647 -1.32216
H -3.73970 4.17402 -1.84854
H -0.87138 3.39067 -1.07145
H -1.47947 3.55316 -2.70790
H -1.26598 1.21601 -2.12961
H -2.98090 1.57559 -2.37412
H -1.61209 1.50966 0.35568
H -1.14201 -2.82906 -0.03092
H -1.56264 -3.57886 2.40130
H -0.48646 -2.28197 2.95892
H 0.16802 -3.62757 2.00327
H -6.31916 -0.85637 -1.63843
H -6.24813 -2.59362 -2.08793
H -4.96519 -1.47168 -2.65649
H -1.66040 -0.41352 1.80990
H -2.18453 -0.84930 -1.20041
H 0.09299 4.31476 2.76143
H 6.19518 -0.24083 2.89055
H 6.26255 2.41253 2.13518
C 5.47669 0.30802 2.29576
C 5.54966 1.62407 1.93973
C 0.64980 4.08077 1.86590
O 0.92637 2.76428 1.66902
C 4.26306 -0.19302 1.72225
O 4.47400 1.97611 1.18668
C 1.15773 4.82973 0.84450
H 1.08569 5.90444 0.73614
H 3.87295 -1.20171 1.75563
C 3.68075 0.85101 1.05403
C 1.64294 2.65484 0.49724
C 1.80419 3.90589 -0.04113
P 2.12910 0.92708 0.07524
Pd 0.68749 -0.89044 0.33700
H 2.34511 4.13385 -0.94722
I 2.47904 -3.07900 -0.26952
C 2.76679 1.17636 -1.62384
O 3.58055 2.24125 -1.97019
C 3.93530 2.07189 -3.27334
C 2.63001 0.34820 -2.70613
H 4.57430 2.83845 -3.68822
H 2.08701 -0.58731 -2.70222
C 3.38386 0.92967 -3.77677
H 3.50593 0.54209 -4.77959

PD_{anti}

B3LYP/6-31+G*/LanL2DZ, E= -1225.700211 A.U.

Thermal correction to Gibbs Free Energy= 0.297732 A.U.

SP at B3LYP/6-311++G**/SDD, E= -1225.918627 A.U.

0 1

C 2.01278 -2.89992 -0.75185
C 0.67859 -2.54256 -0.53670
C 0.40142 -1.19446 -0.29857
C 1.41753 -0.23081 -0.29298
C 2.75032 -0.58724 -0.52286
C 3.03254 -1.94489 -0.74562
C 3.85603 0.44795 -0.54809
C 3.97612 1.32676 0.71525
C 2.90792 2.42360 0.86042
C 1.46903 1.94129 1.09782
C 0.84933 1.15264 -0.07098
C -0.68156 0.90842 0.14159
C -1.54405 1.74376 -0.76425
C -2.47073 2.60962 -0.33577
C -3.31040 3.48934 -1.21783
N -0.86567 -0.56378 -0.11356
C -3.40281 -1.36946 -0.74239
S -2.20971 -1.32377 0.60750
O -1.85837 -2.70900 0.93563
O -2.74425 -0.42375 1.63792
H 2.25672 -3.94500 -0.92539
H -0.10224 -3.29150 -0.52531
H 4.06075 -2.25383 -0.91969
H 3.72174 1.10862 -1.42007
H 4.80872 -0.07120 -0.70864
H 4.95932 1.81639 0.69117
H 3.97188 0.68310 1.60628
H 2.92867 3.06213 -0.03678
H 3.19152 3.07326 1.69972
H 0.83673 2.82064 1.28693
H 1.42693 1.32270 2.00564
H 0.98079 1.75215 -0.98580
H -0.94820 1.11108 1.18337
H -1.35744 1.62785 -1.83471
H -2.64658 2.69305 0.73817
H -4.38074 3.29877 -1.06006
H -3.08607 3.33337 -2.27903
H -3.14487 4.55056 -0.98715
H -3.60254 -0.34553 -1.06232
H -4.30805 -1.83757 -0.34685
H -2.98359 -1.96444 -1.55612

PD_{syn}

B3LYP/6-31+G*/LanL2DZ, E= -1225.690228 A.U.

Thermal correction to Gibbs Free Energy= 0.299636 A.U.

SP at B3LYP/6-311++G**/SDD, E= -1225.908716 A.U.

0 1

C 2.63330 -2.48052 -0.76789
C 1.23743 -2.41651 -0.75053
C 0.65190 -1.15718 -0.61132
C 1.42715 0.00371 -0.53758
C 2.82310 -0.06035 -0.51419
C 3.41496 -1.32605 -0.63941
C 3.64052 1.19083 -0.27964
C 3.31140 1.89997 1.05608
C 1.99928 2.70820 1.08904
C 0.67590 1.93263 0.93502
C 0.55468 1.23121 -0.43216
C -0.83930 0.64765 -0.85110
C -2.04352 1.38747 -0.34321
C -2.89139 2.03080 -1.15762
C -4.06088 2.85895 -0.70654
N -0.75449 -0.84696 -0.57141
C -3.28261 -1.72530 -0.04422
S -1.65713 -1.55874 0.71537
O -1.11749 -2.90809 0.91592
O -1.78040 -0.65265 1.87029
H 3.11878 -3.44769 -0.87008
H 0.63229 -3.31214 -0.81351
H 4.49960 -1.41071 -0.63107
H 3.49519 1.90394 -1.10642
H 4.70460 0.92487 -0.28799
H 4.13141 2.59635 1.27978
H 3.30926 1.15434 1.86337
H 2.04476 3.47917 0.30334
H 1.96279 3.25313 2.04226
H -0.14487 2.65361 1.04238
H 0.56039 1.19952 1.74352
H 0.82416 1.96926 -1.20183
H -0.86833 0.68315 -1.94710
H -2.18667 1.43620 0.73324
H -2.73514 1.96964 -2.23743
H -4.99966 2.48636 -1.13902
H -3.95579 3.90076 -1.03911
H -4.16061 2.85789 0.38421
H -3.92381 -2.17814 0.71636
H -3.18760 -2.37860 -0.91270
H -3.65365 -0.73936 -0.32615

TFP

B3LYP/6-31+G*/LanL2DZ, E= -1029.652308 A.U.

Thermal correction to Gibbs Free Energy= 0.13902 A.U.

SP at B3LYP/6-311++G**/SDD, E= -1029.837013 A.U.

0 1

P -0.00013 -0.00023 -1.07159

C 2.82954 -2.51640 -0.09521

C 3.10001 -1.69008 0.95573

C 2.14509 -0.62453 0.87852

C 1.35652 -0.87618 -0.21382

O 1.78388 -2.03656 -0.82184

C -3.59419 -1.19179 -0.09469

C -3.01383 -1.83934 0.95616

C -1.61350 -1.54555 0.87872

C -1.43709 -0.73685 -0.21365

O -2.65573 -0.52641 -0.82148

C 0.08038 1.61278 -0.21413

C -0.53189 2.17032 0.87796

C -0.08610 3.52993 0.95501

C 0.76504 3.70837 -0.09579

O 0.87208 2.56270 -0.82217

H 3.26545 -3.43741 -0.45303

H 3.88125 -1.82011 1.69264

H 2.05141 0.22290 1.54366

H -4.60978 -1.10852 -0.45236

H -3.51711 -2.45077 1.69314

H -0.83276 -1.88834 1.54375

H -1.21927 1.66586 1.54307

H -0.36401 4.27177 1.69170

H 1.34506 4.54610 -0.45365

I^-

B3LYP/6-31+G*/LanL2DZ, E= -11.47211005 A.U.

Thermal correction to Gibbs Free Energy= -0.016848 A.U.

SP at B3LYP/6-311++G**/SDD, E= -11.51890909 A.U.

-1 1

I 0.00000 0.00000 0.00000

Pd(TFP)$_2$

B3LYP/6-31+G*/LanL2DZ, E= -2186.089036 A.U.

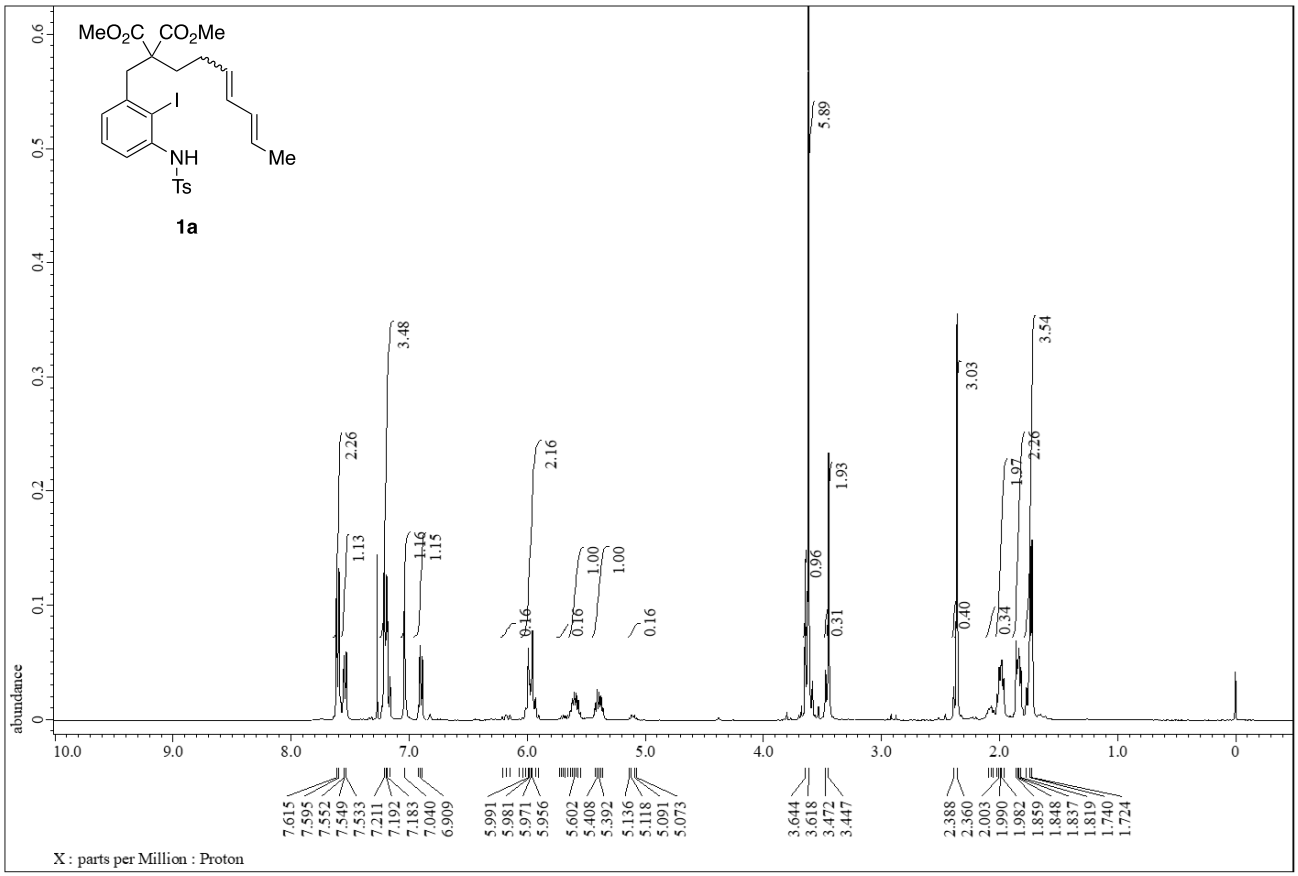
Thermal correction to Gibbs Free Energy= 0.291562 A.U.

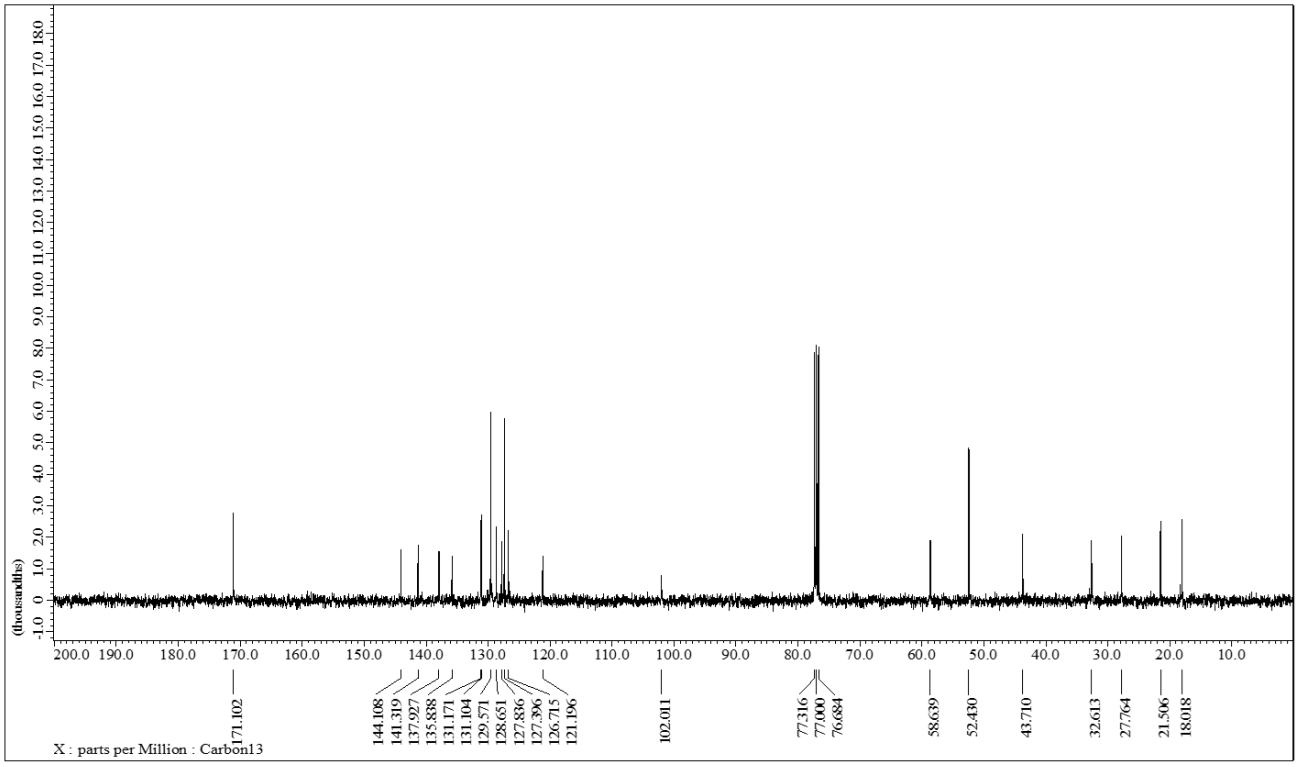
SP at B3LYP/6-311++G**/SDD, E= -2187.664372 A.U.

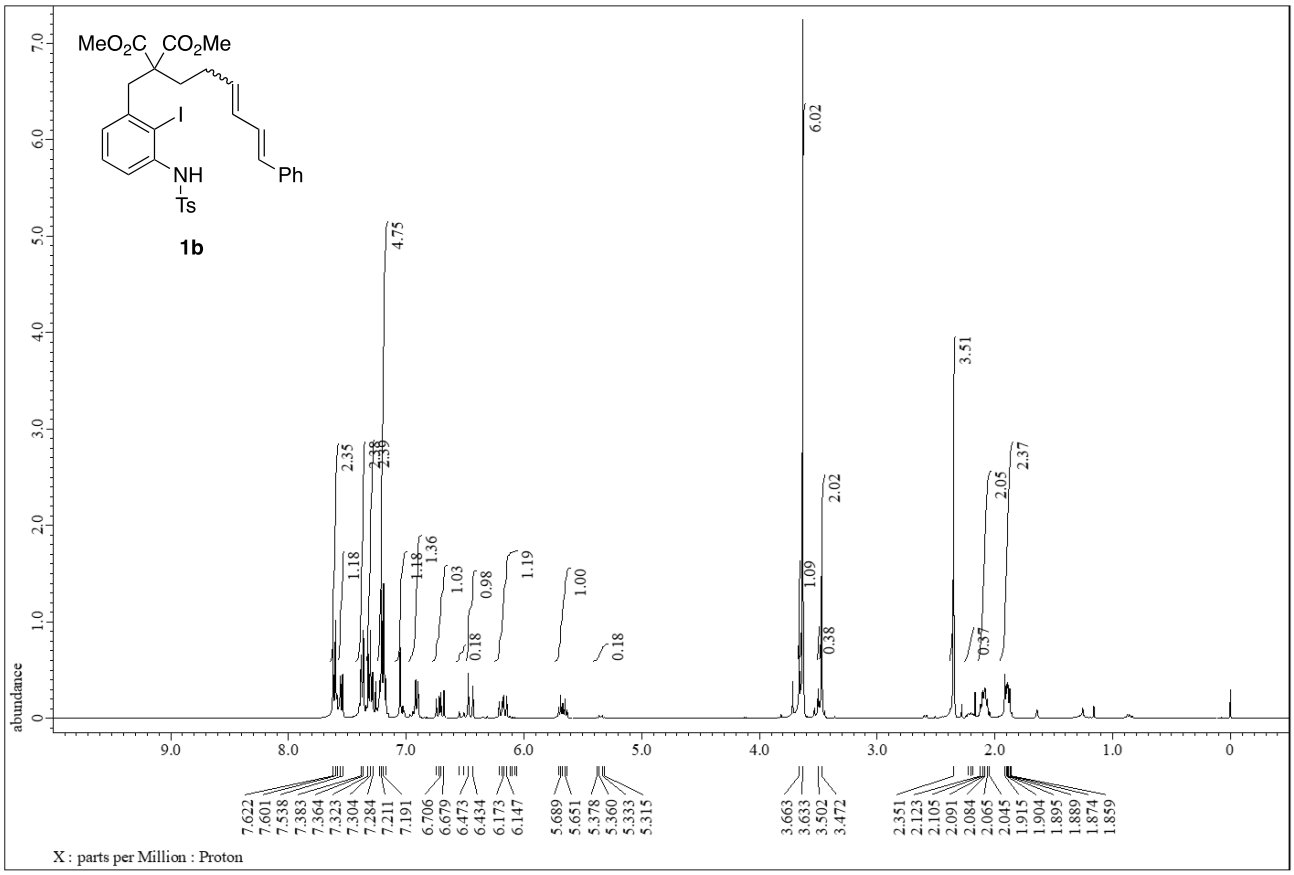
0 1

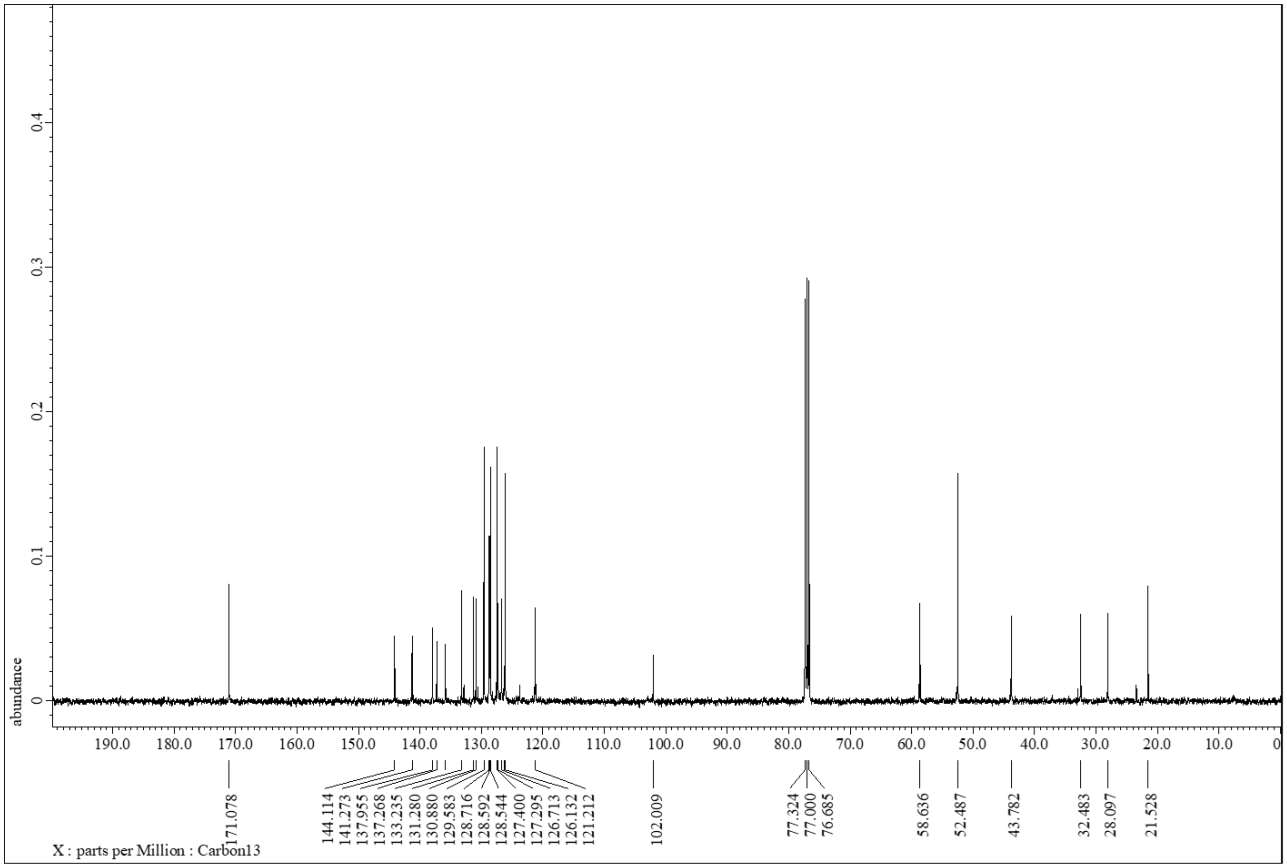
Pd 0.00000 0.00017 0.14048
P 2.30844 0.00170 0.01643
C 3.26984 -0.07594 1.56706
C 4.37725 -0.77182 1.97584
C 4.59986 -0.42130 3.34693
C 3.61426 0.46367 3.67502
O 2.79457 0.67996 2.61158
C 2.99999 1.46023 -0.81927
C 3.09812 -1.35799 -0.91129
C 3.37493 3.39913 -1.89949
C 4.56490 2.84219 -1.53015
O 4.36253 1.66745 -0.87419
O 2.57659 -2.61238 -0.69515
C 3.25660 -3.47961 -1.49251
C 4.19674 -2.81708 -2.22638
C 4.09612 -1.43867 -1.84757
C 2.35938 2.50373 -1.43390
H 4.96234 -1.44725 1.36741
H 5.38650 -0.78011 3.99704
H 3.36319 1.00237 4.57669
H 3.23740 4.33216 -2.42895
H 5.59631 3.14218 -1.64587
H 2.95542 -4.51436 -1.42261
H 4.87758 -3.25174 -2.94589
H 4.68994 -0.61344 -2.21343
H 1.28705 2.60732 -1.52786
P -2.30845 -0.00154 0.01640
C -3.26979 0.07574 1.56709
C -4.37730 0.77140 1.97601
C -4.59978 0.42069 3.34707
C -3.61401 -0.46415 3.67502
O -2.79434 -0.68019 2.61151
C -2.99972 -1.46014 -0.81941
C -3.09845 1.35808 -0.91112
C -3.37431 -3.39904 -1.89975
C -4.56439 -2.84233 -1.53040
O -4.36222 -1.66760 -0.87436
O -2.57693 2.61250 -0.69512
C -3.25722 3.47970 -1.49226
C -4.19755 2.81714 -2.22586
C -4.09673 1.43873 -1.84710
C -2.35892 -2.50349 -1.43410
H -4.96253 1.44680 1.36769
H -5.38644 0.77931 3.99726
H -3.36280 -1.00291 4.57662
H -3.23661 -4.33201 -2.42927
H -5.59574 -3.14249 -1.64616
H -2.95607 4.51447 -1.42243
H -4.87862 3.25177 -2.94515
H -4.69062 0.61347 -2.21280
H -1.28658 -2.60689 -1.52805

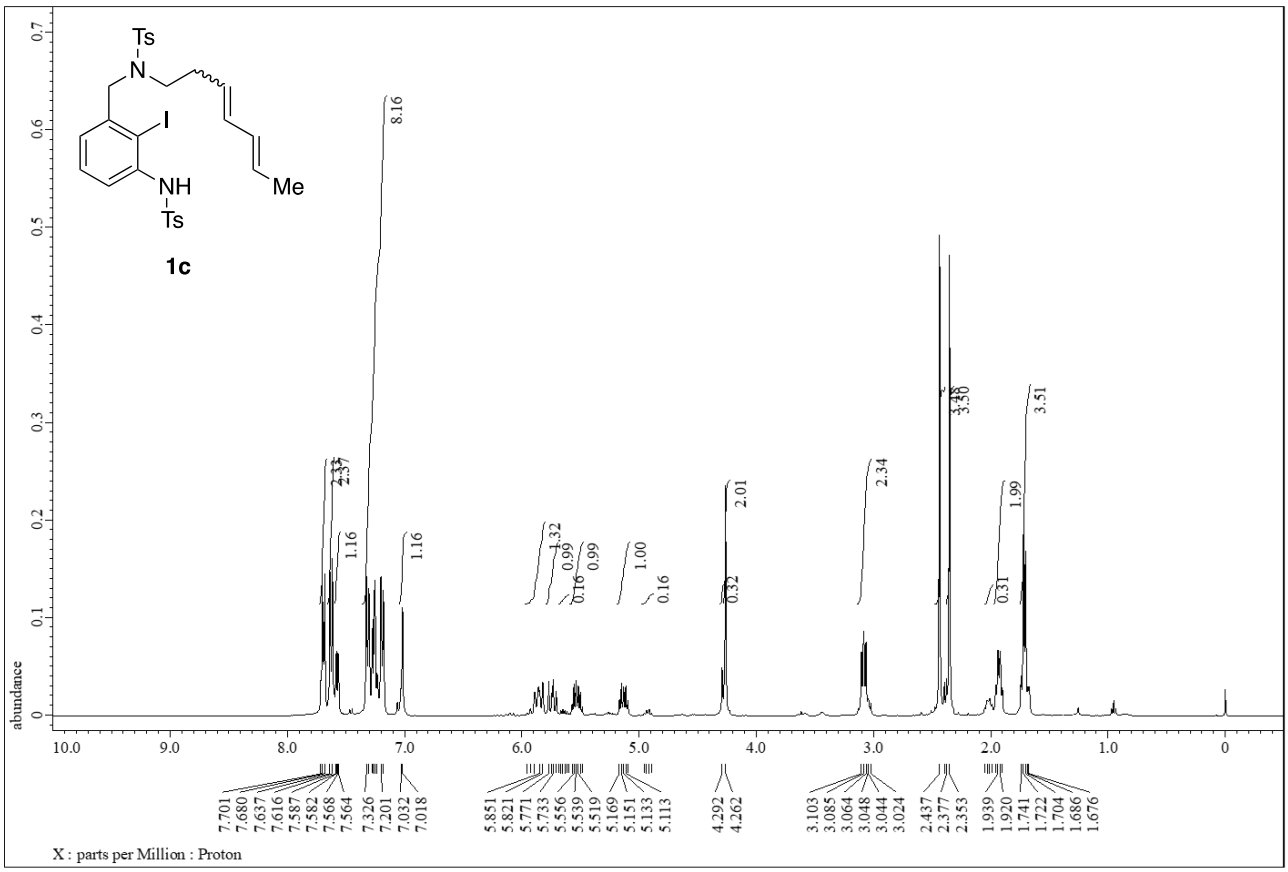
2. ^{1}H and ^{13}C NMR Spectra

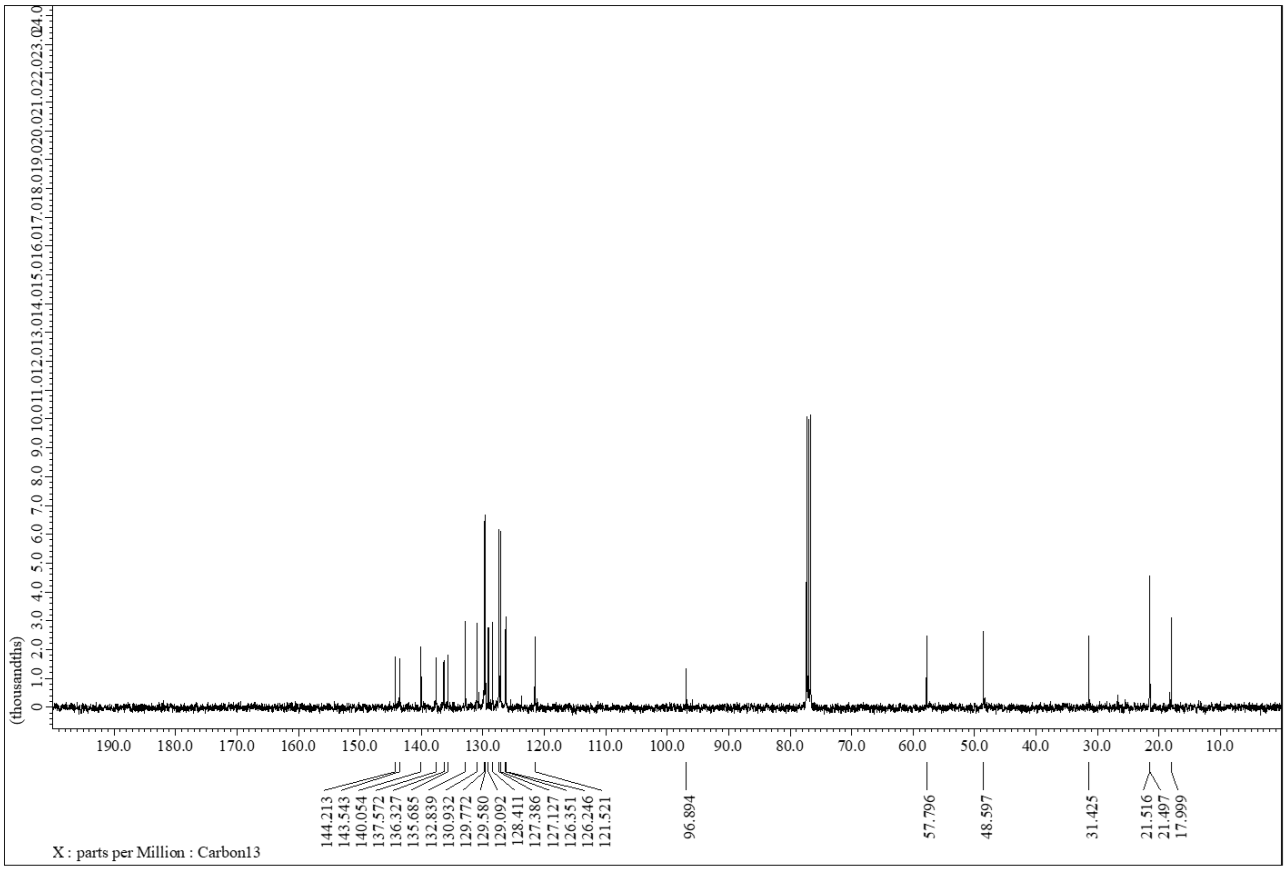


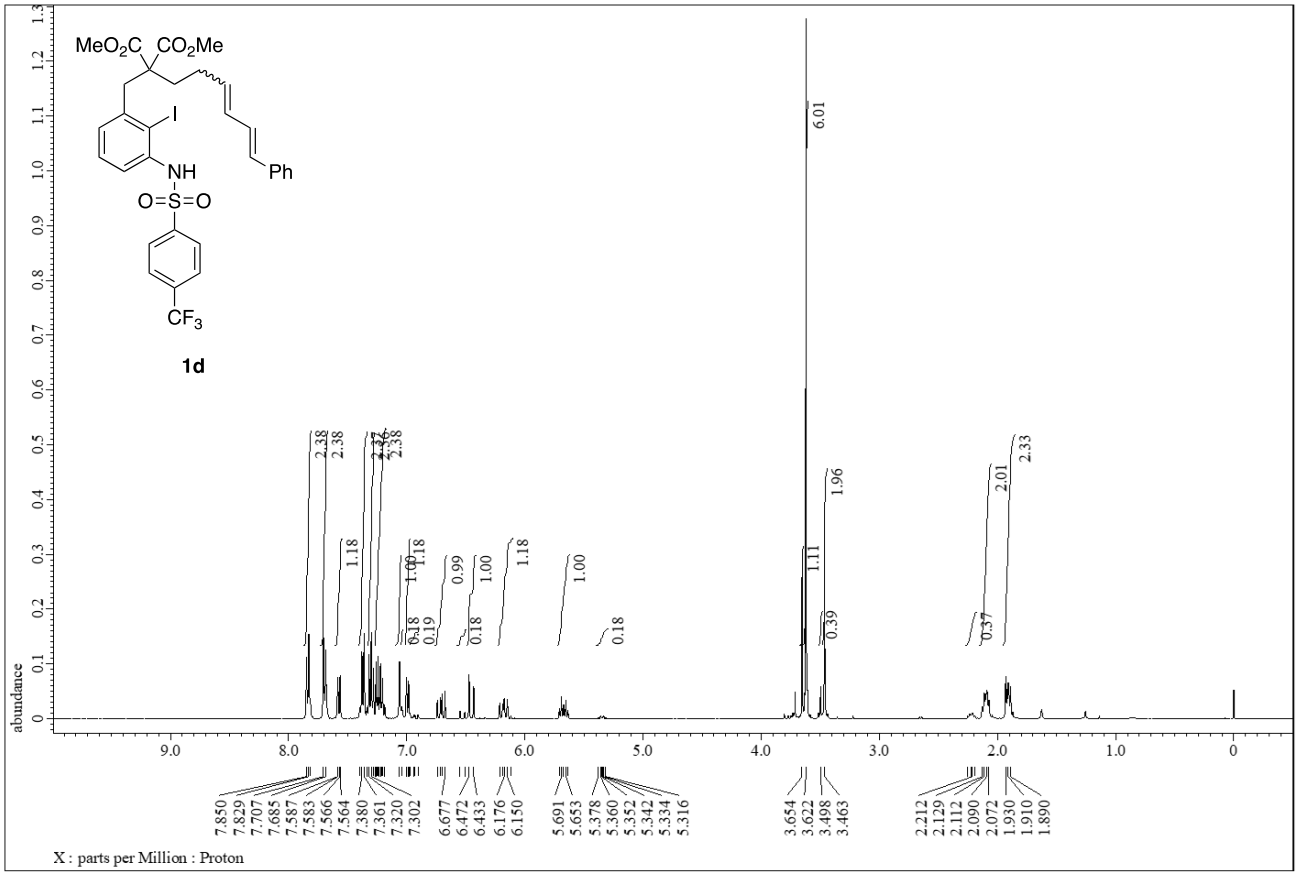


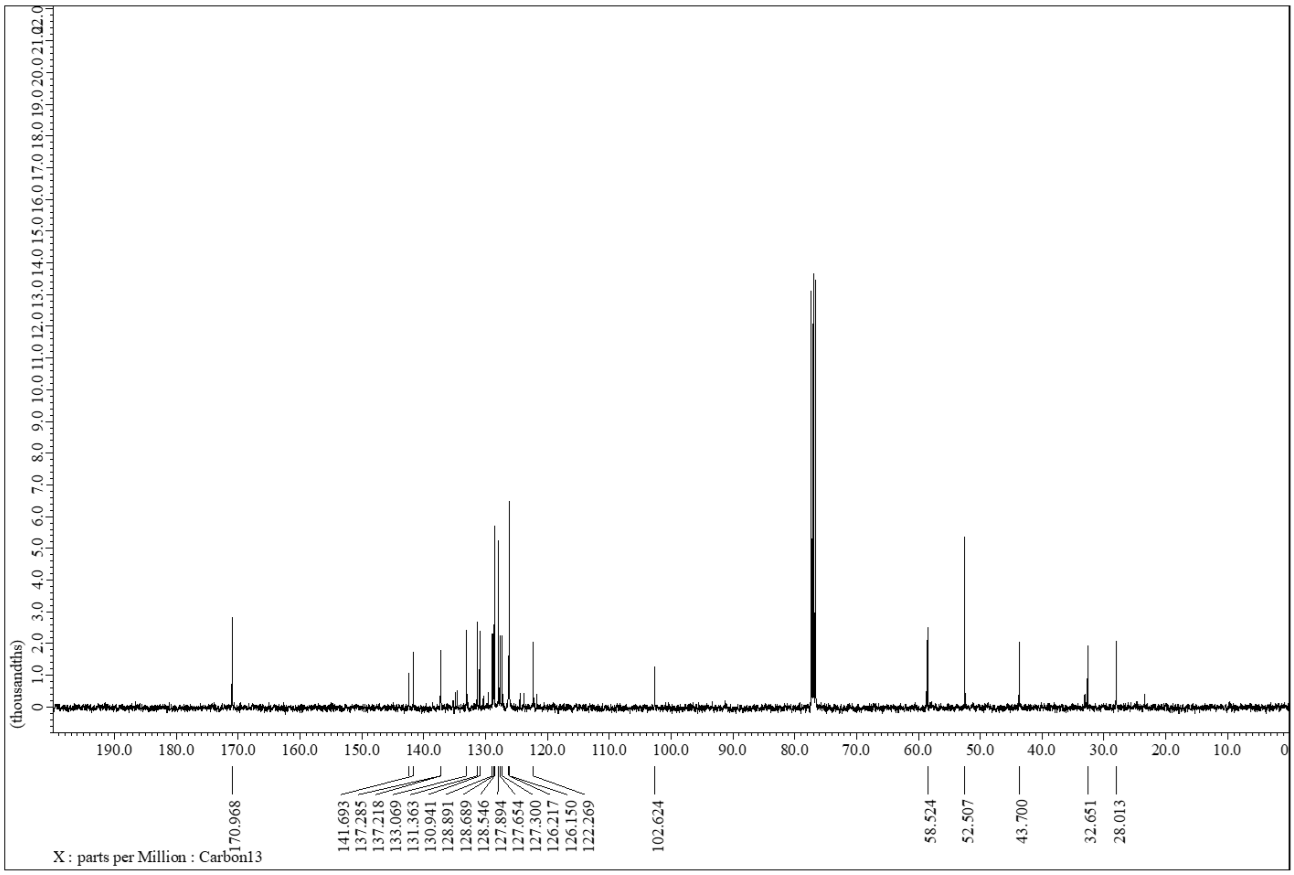

MeO2C CO2Me
I
NH
Ts
Ph
1b
abundance
X : parts per Million : Proton

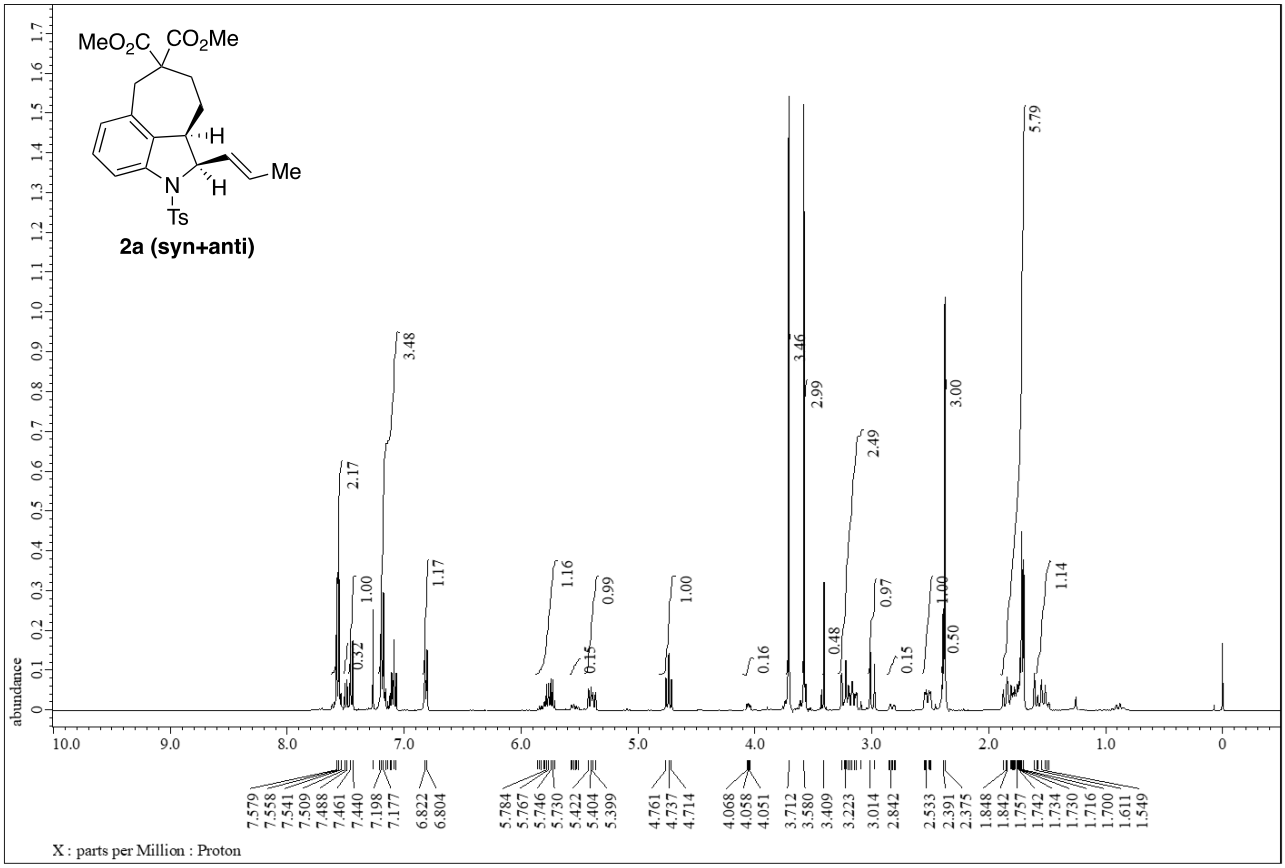

abundance
X : parts per Million : Carbon13

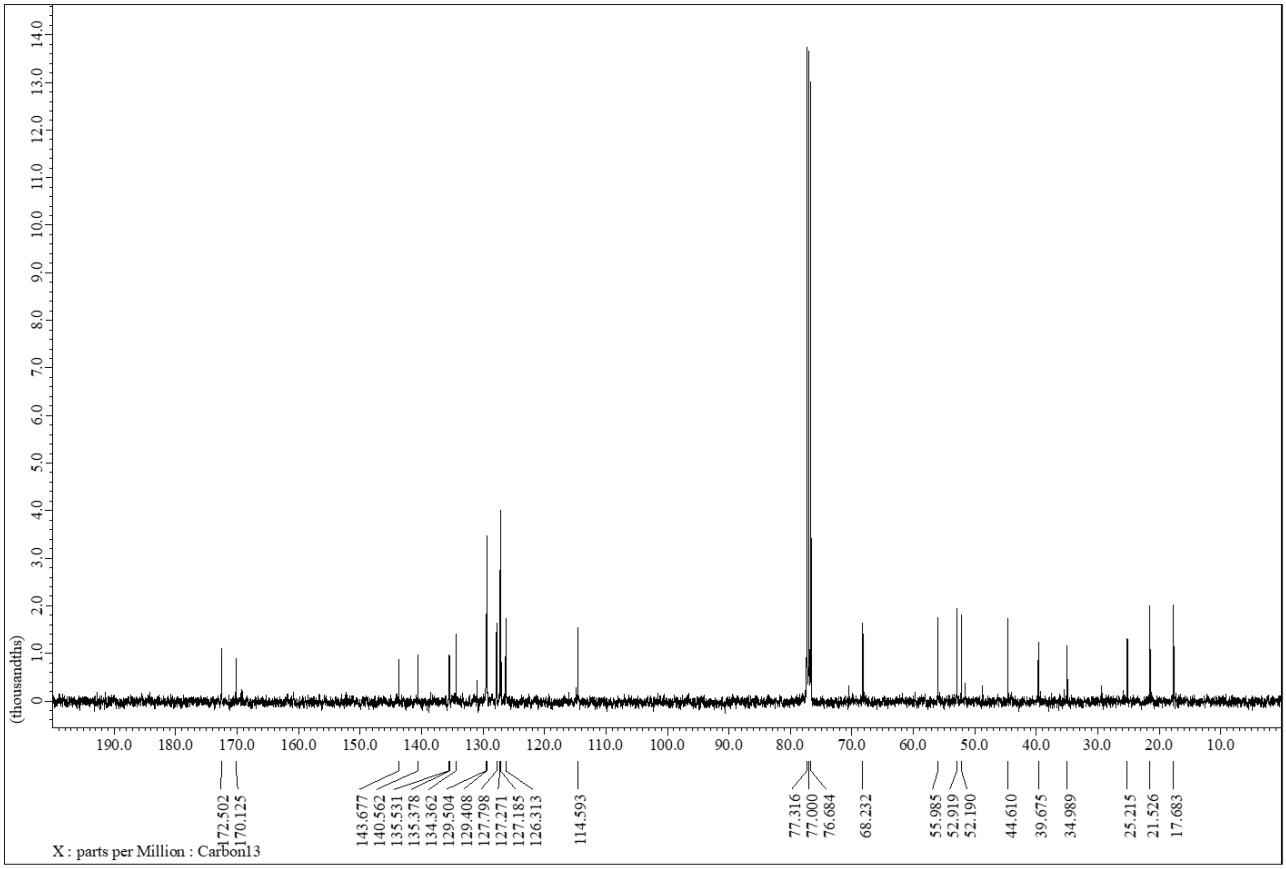

Ts
N
I
NH
Ts
Me
1c
8.16
2.37
2.33
1.16
1.16
4.32
0.99
0.16
0.99
1.00
0.16
0.32
2.01
2.34
3.51
1.99
0.31
abundance
X : parts per Million : Proton

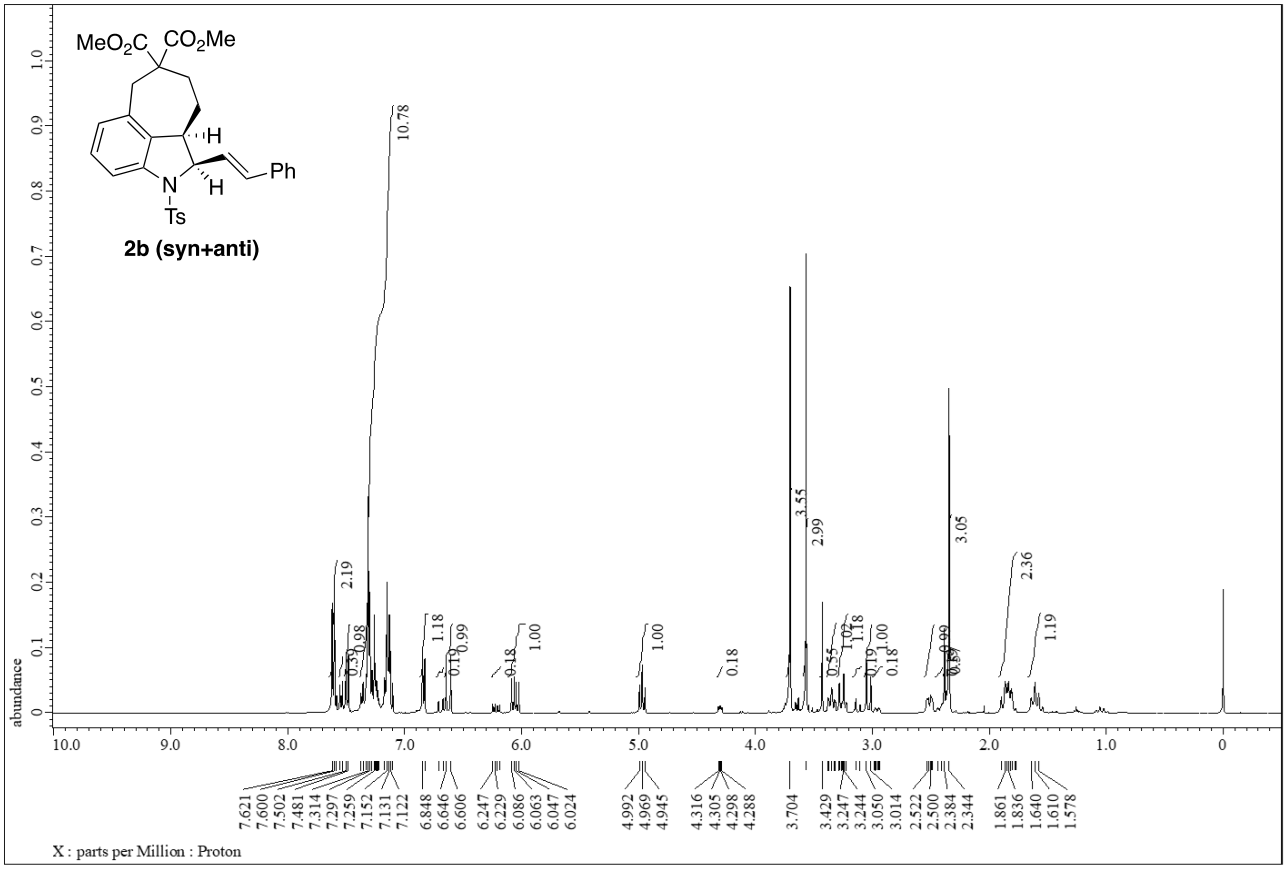

(thousandths)
144.213
143.543
140.054
137.572
136.327
135.685
132.839
130.932
129.772
129.580
129.092
128.411
127.386
127.127
126.351
126.246
121.521
96.894
57.796
48.597
31.425
21.516
21.497
17.999
X : parts per Million : Carbon13

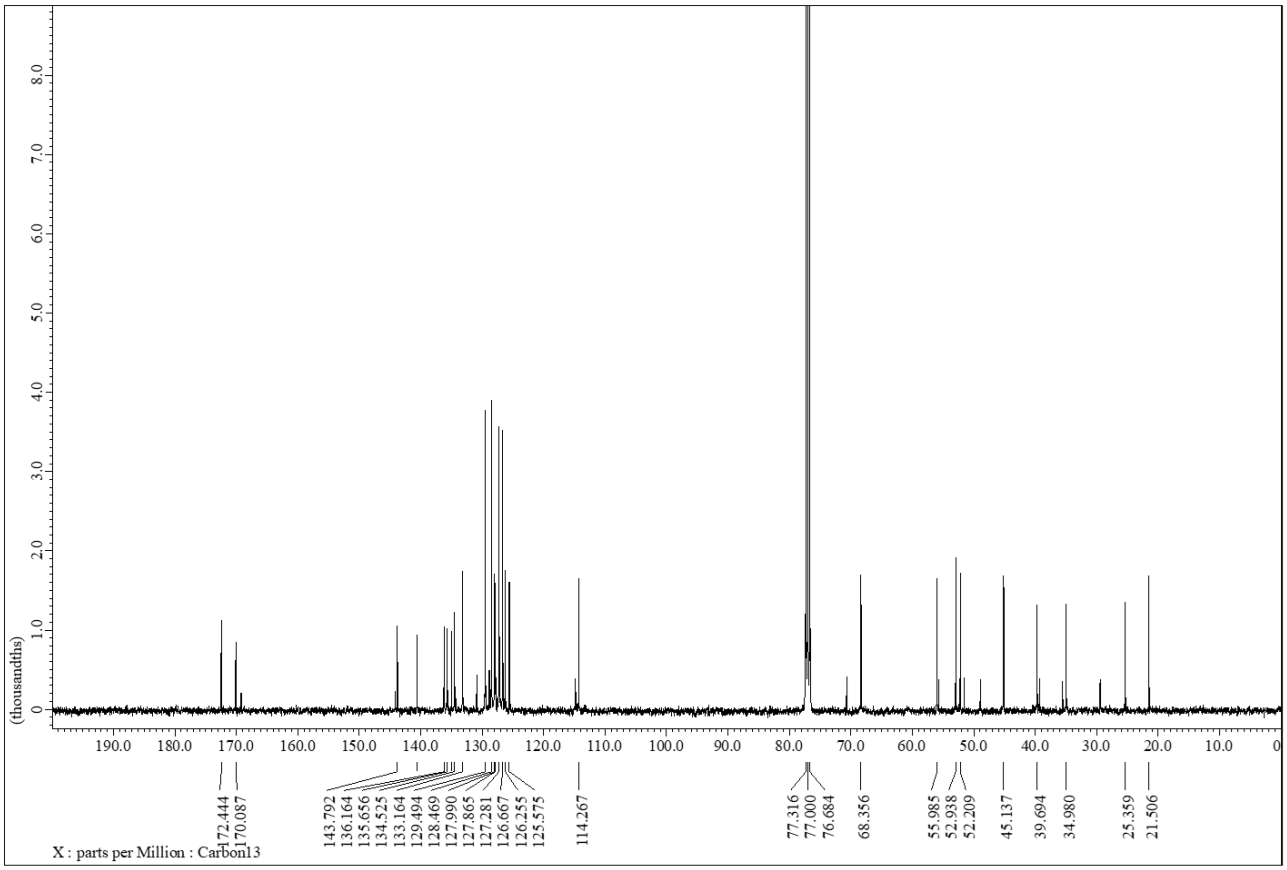

MeO2C CO2Me
I
NH
O=S=O
Ph
CF3
1d
abundance
X : parts per Million : Proton

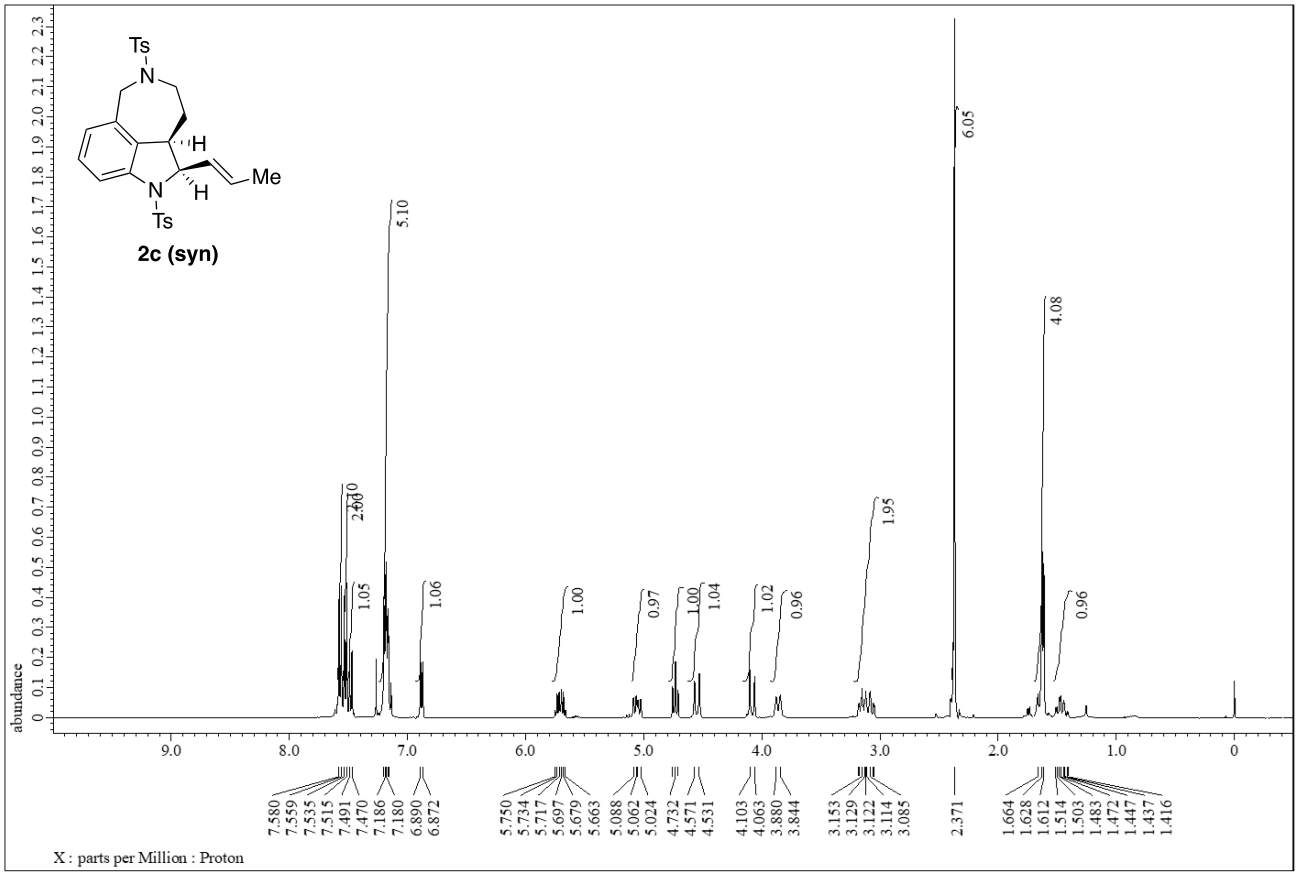

(thousandths)
X : parts per Million : Carbon13

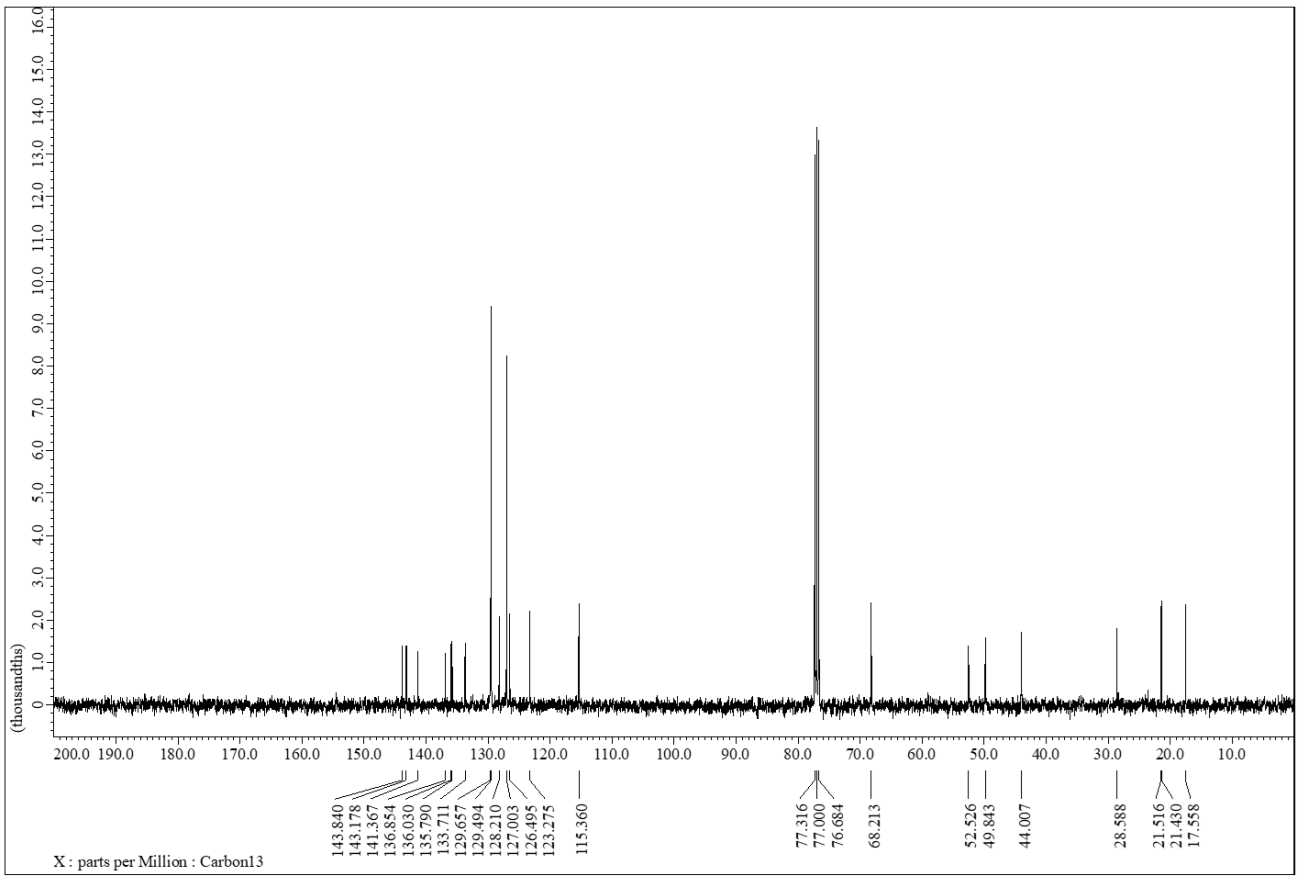

MeO2C
CO2Me
H
Me
N
H
Ts
2a (syn+anti)
abundance
X : parts per Million : Proton

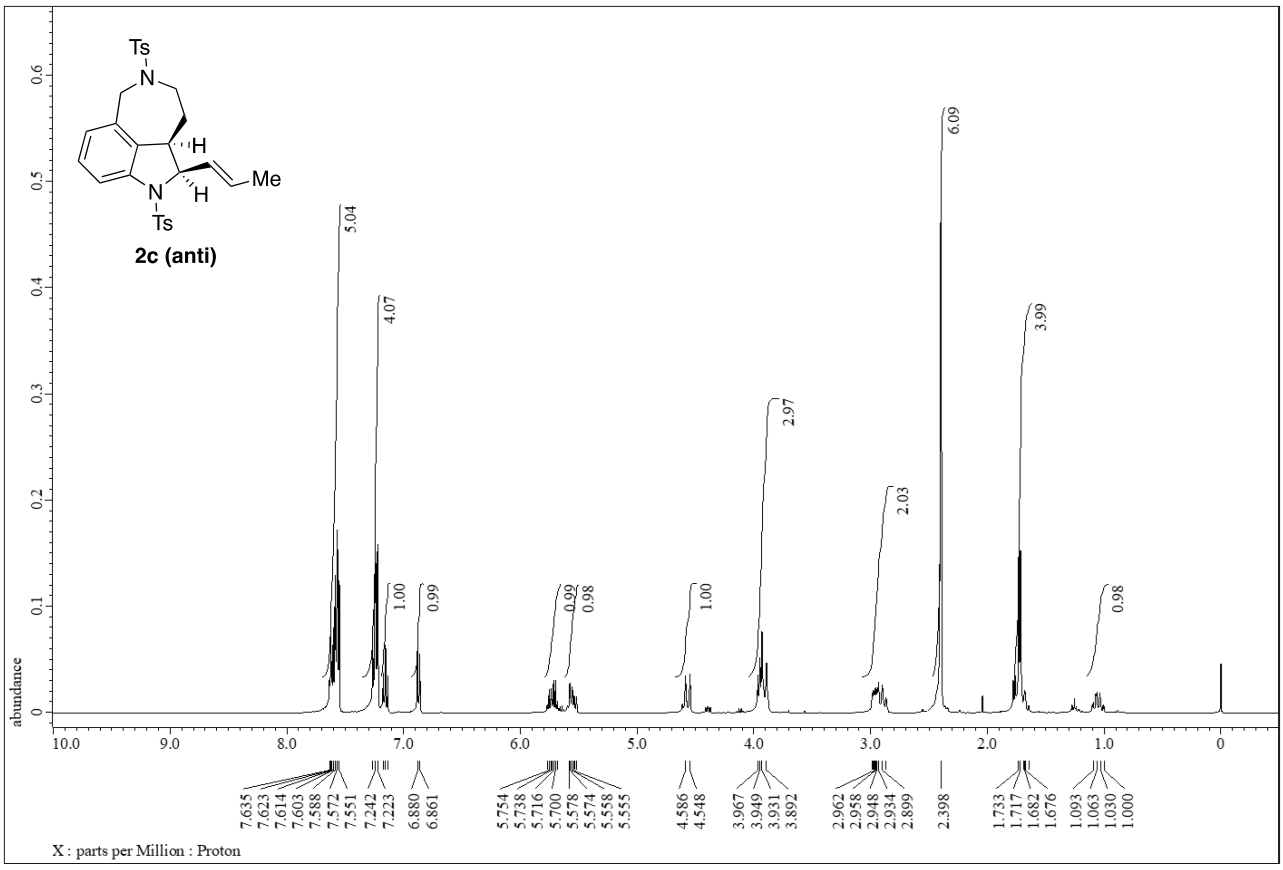

(thousandths)
X : parts per Million : Carbon13

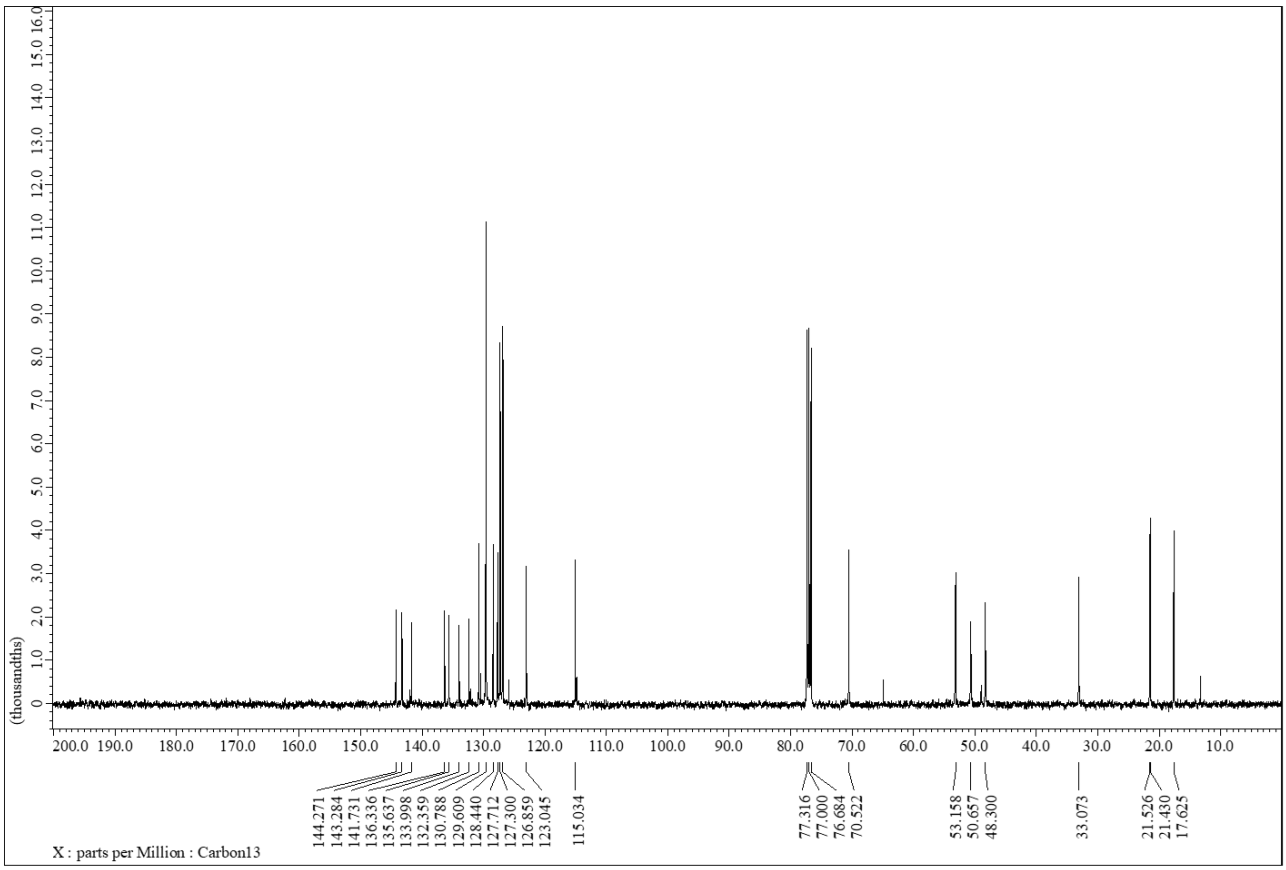

MeO2C
CO2Me
H
Ph
N
H
Ts
2b (syn+anti)
abundance
X : parts per Million : Proton

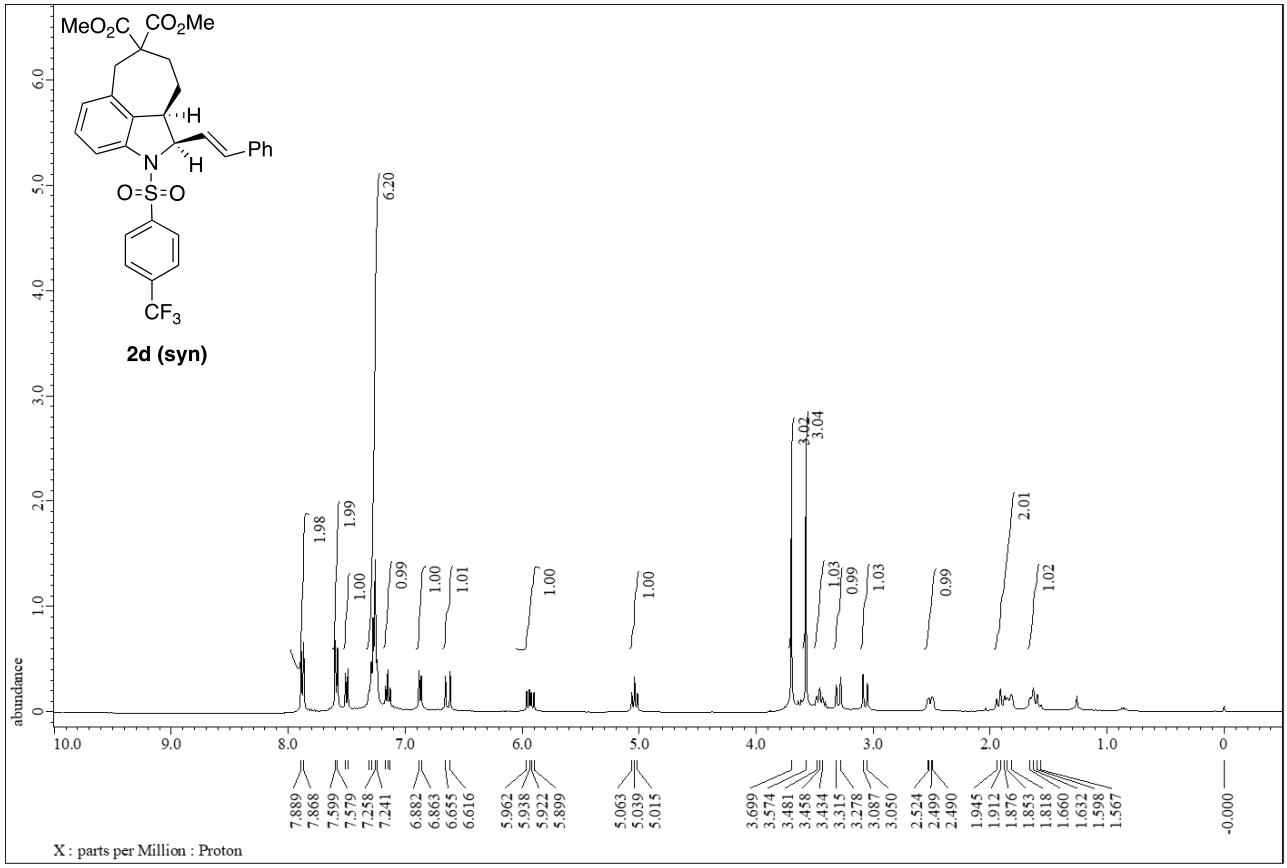

(thousandths)
X : parts per Million : Carbon13

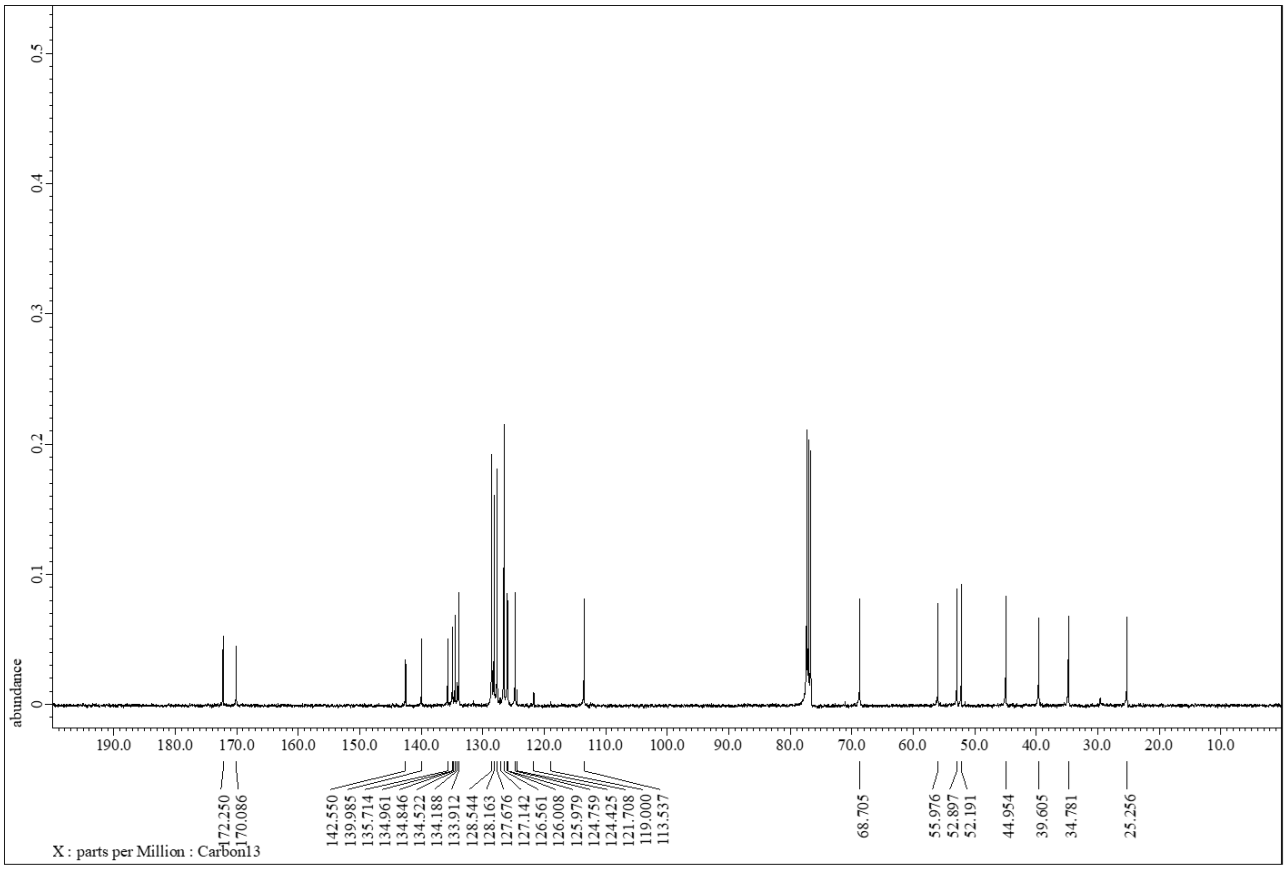

Ts
N
H
Me
N
H
Ts
2c (syn)
abundance
X : parts per Million : Proton

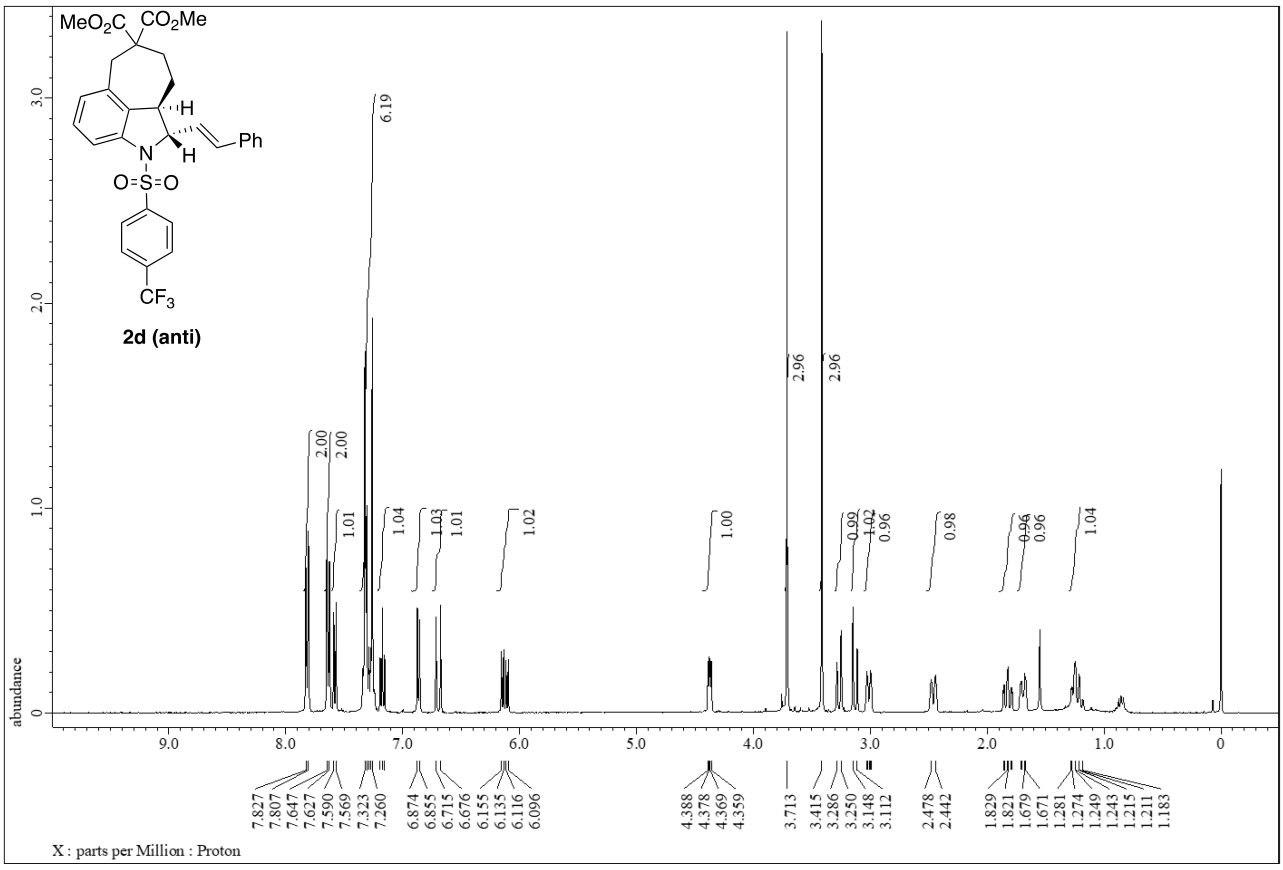

(thousandths)
X : parts per Million : Carbon13

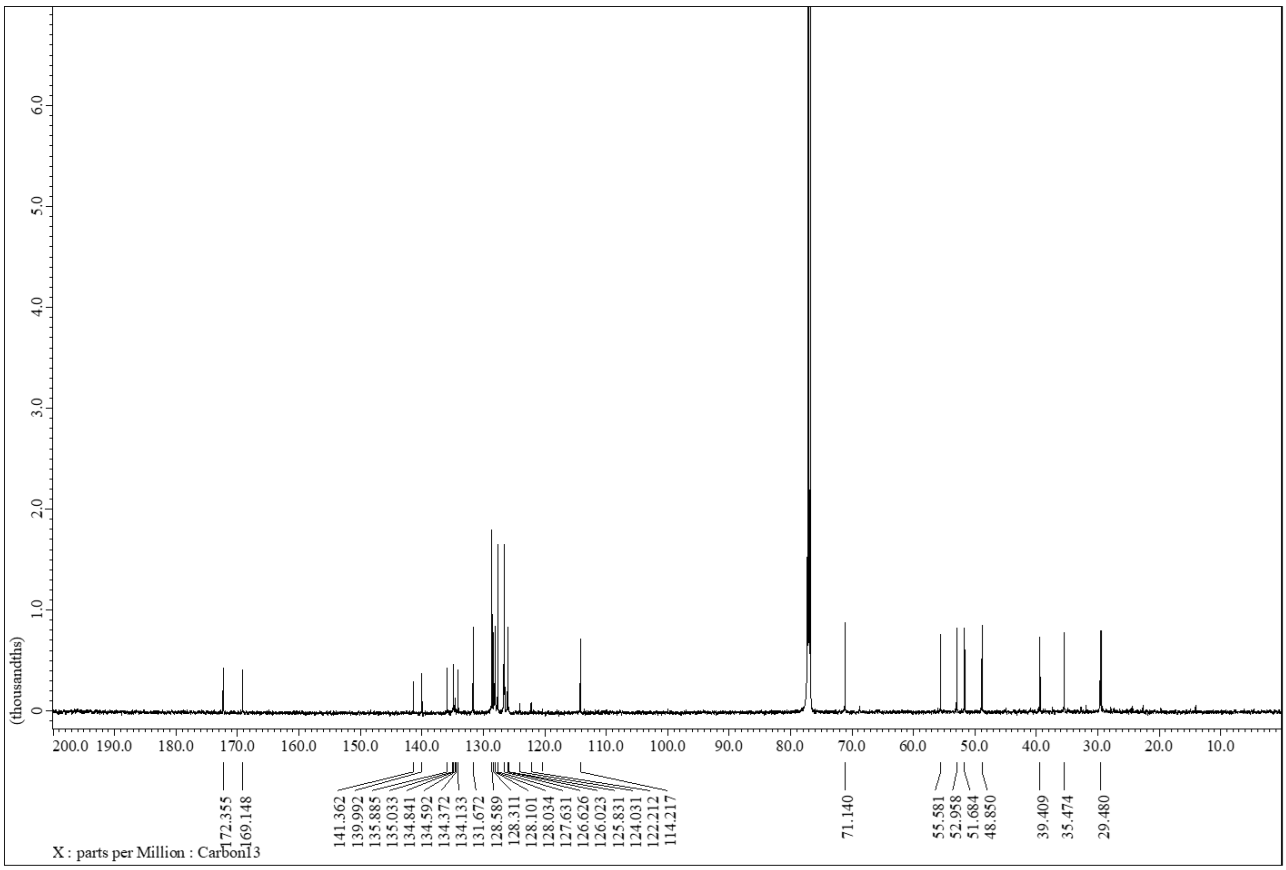

Ts
N
H
Me
N
H
Ts
2c (anti)
abundance
X : parts per Million : Proton

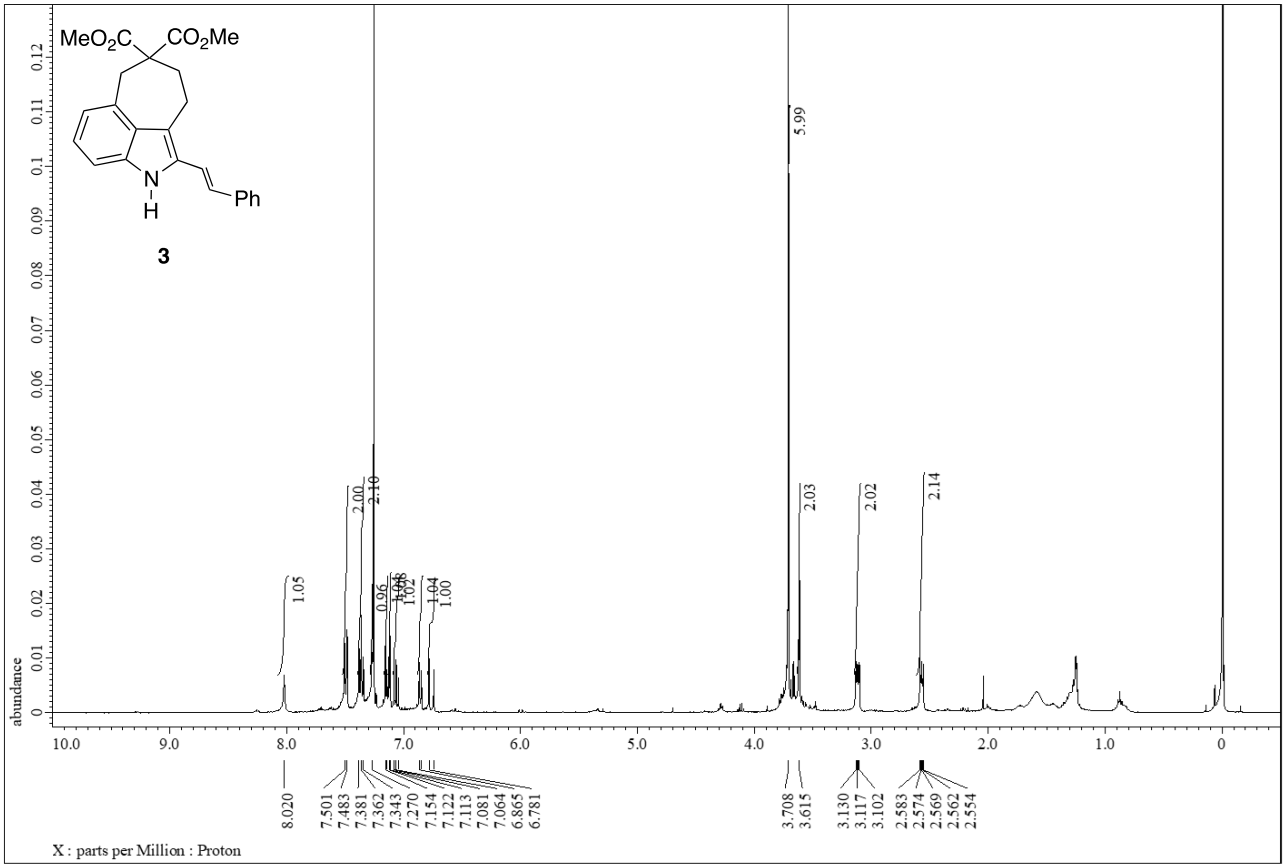

(thousandths)
X : parts per Million : Carbon13

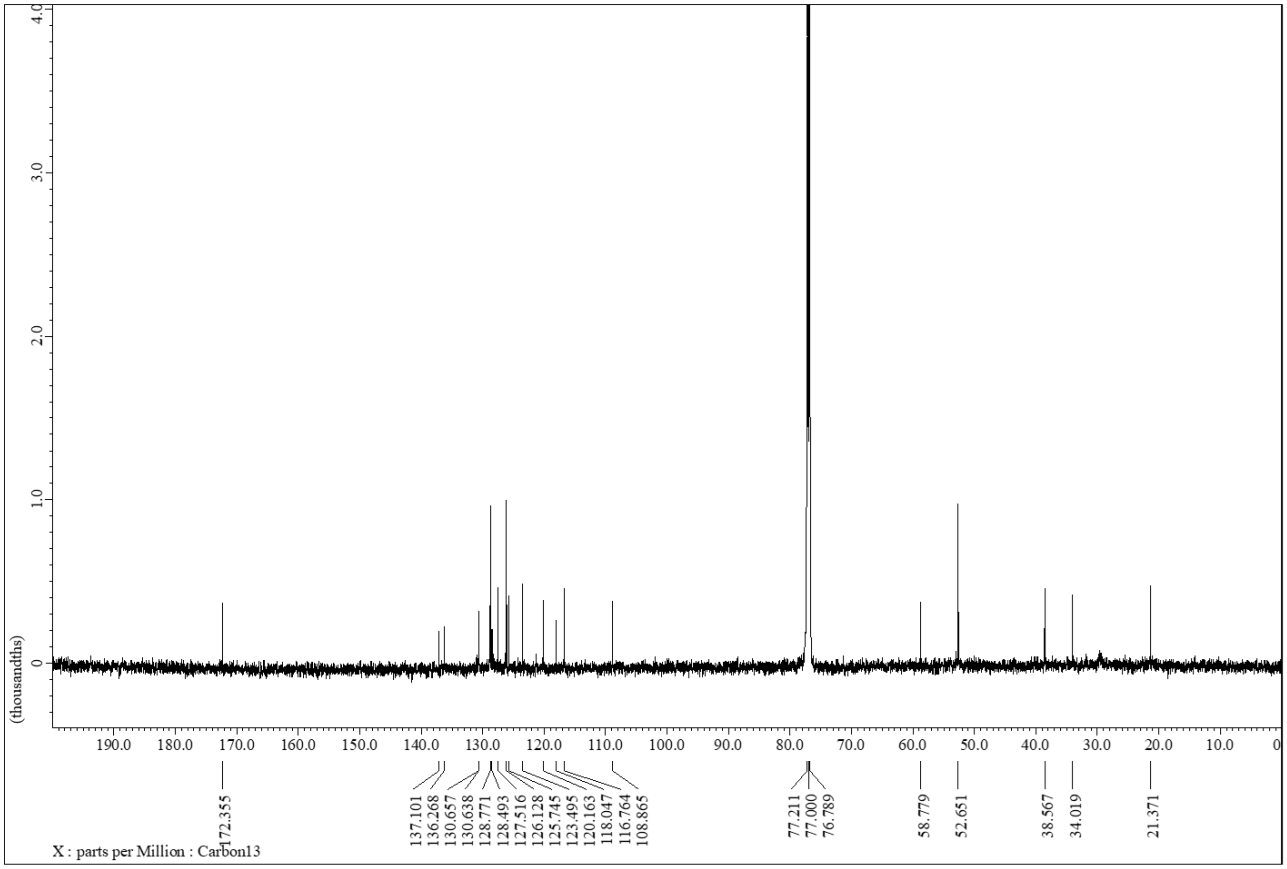

MeO2C
CO2Me
H
Ph
N
H
O=S=O
CF3
2d (syn)
abundance
X : parts per Million : Proton

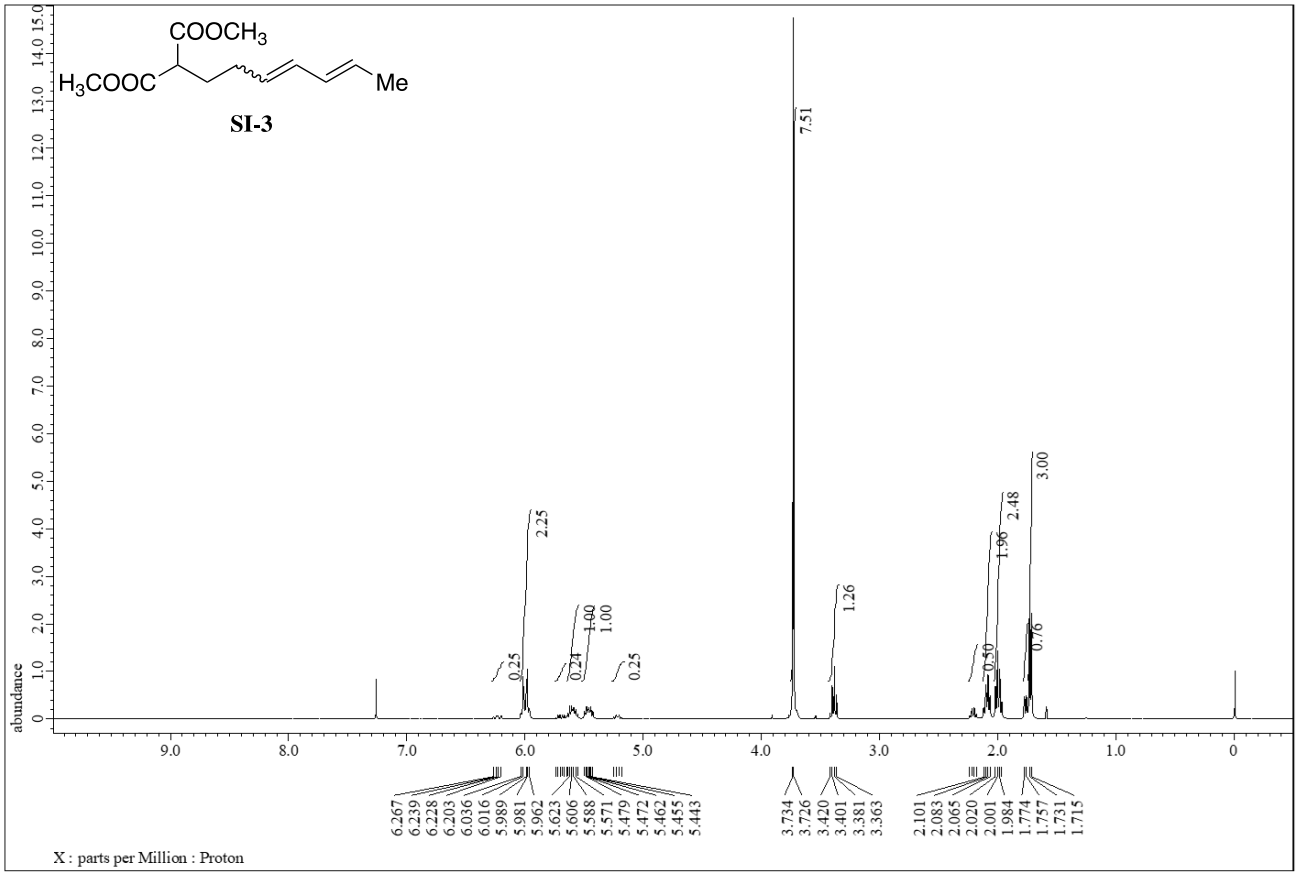

abundance
X : parts per Million : Carbon13

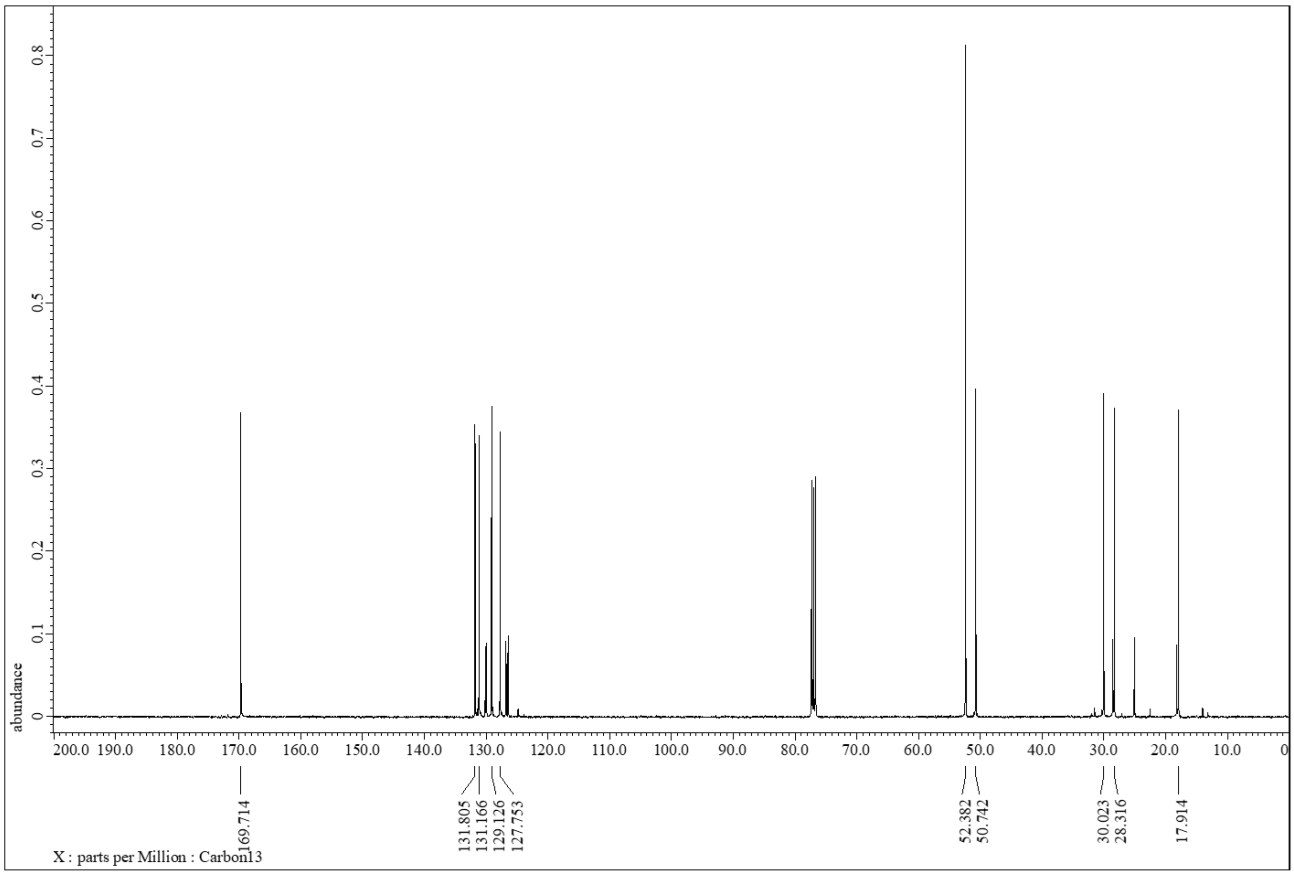

MeO2C CO2Me
H
N
H
Ph
O=S=O
CF3
2d (anti)
abundance
X : parts per Million : Proton

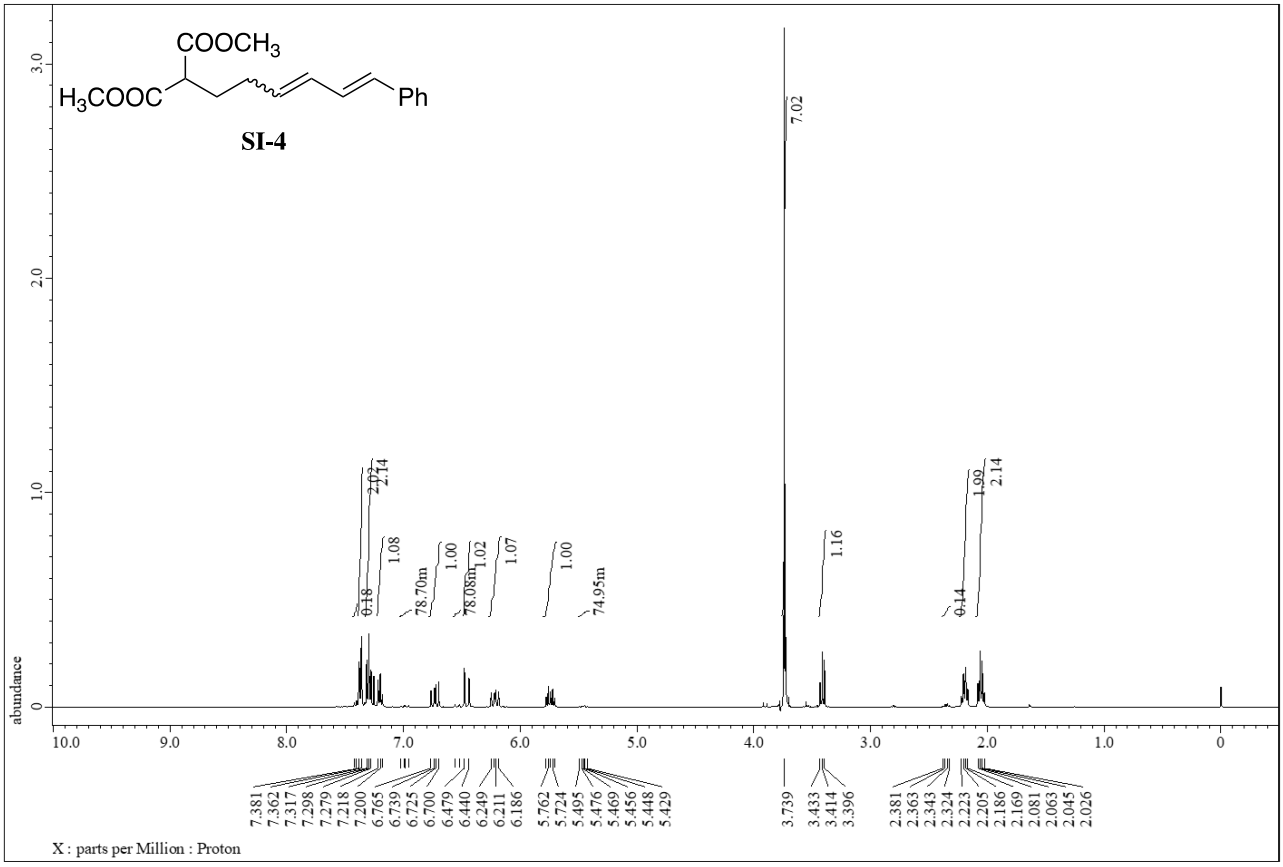

(thousandths)
X : parts per Million : Carbon13

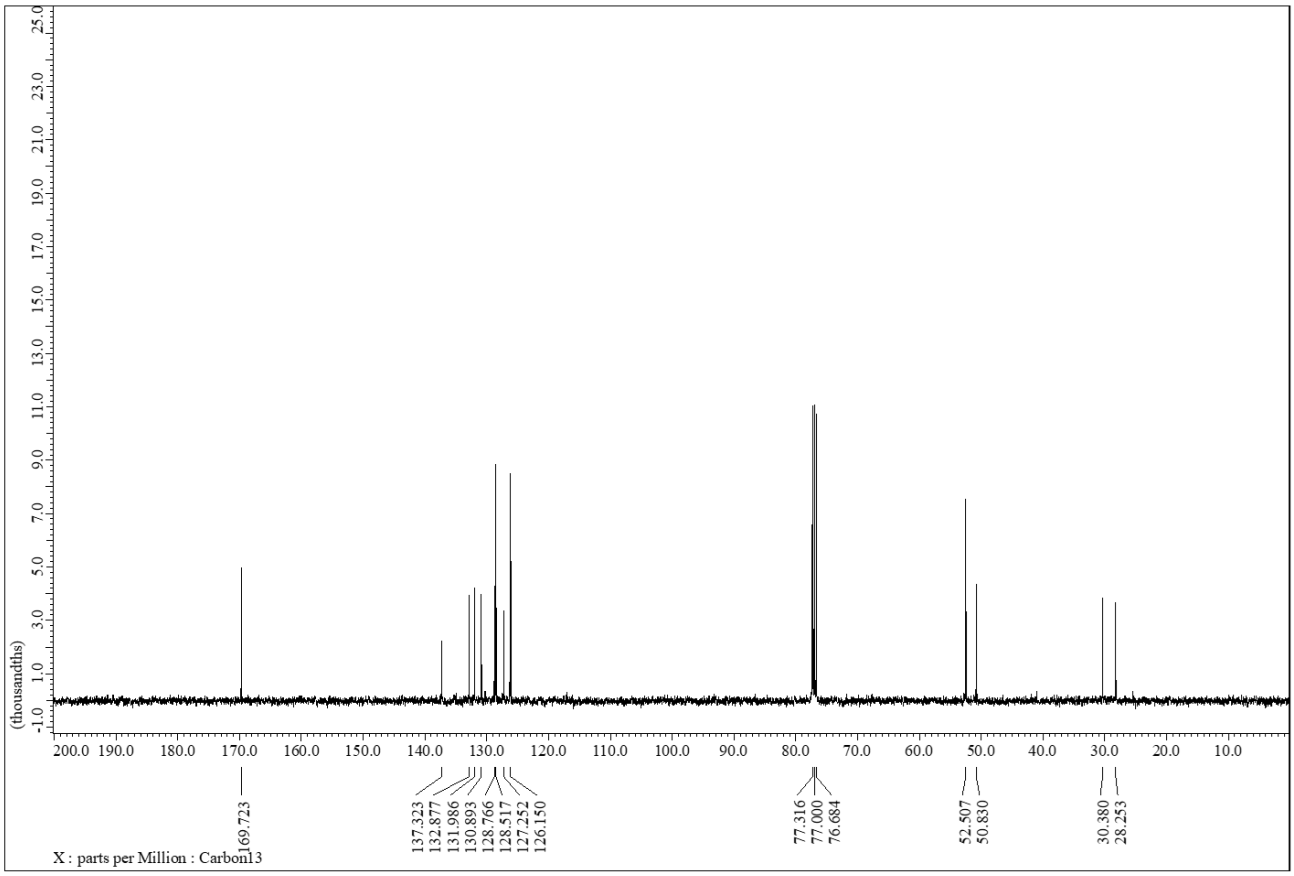

MeO2C
CO2Me
N
H
Ph
3
abundance
X : parts per Million : Proton

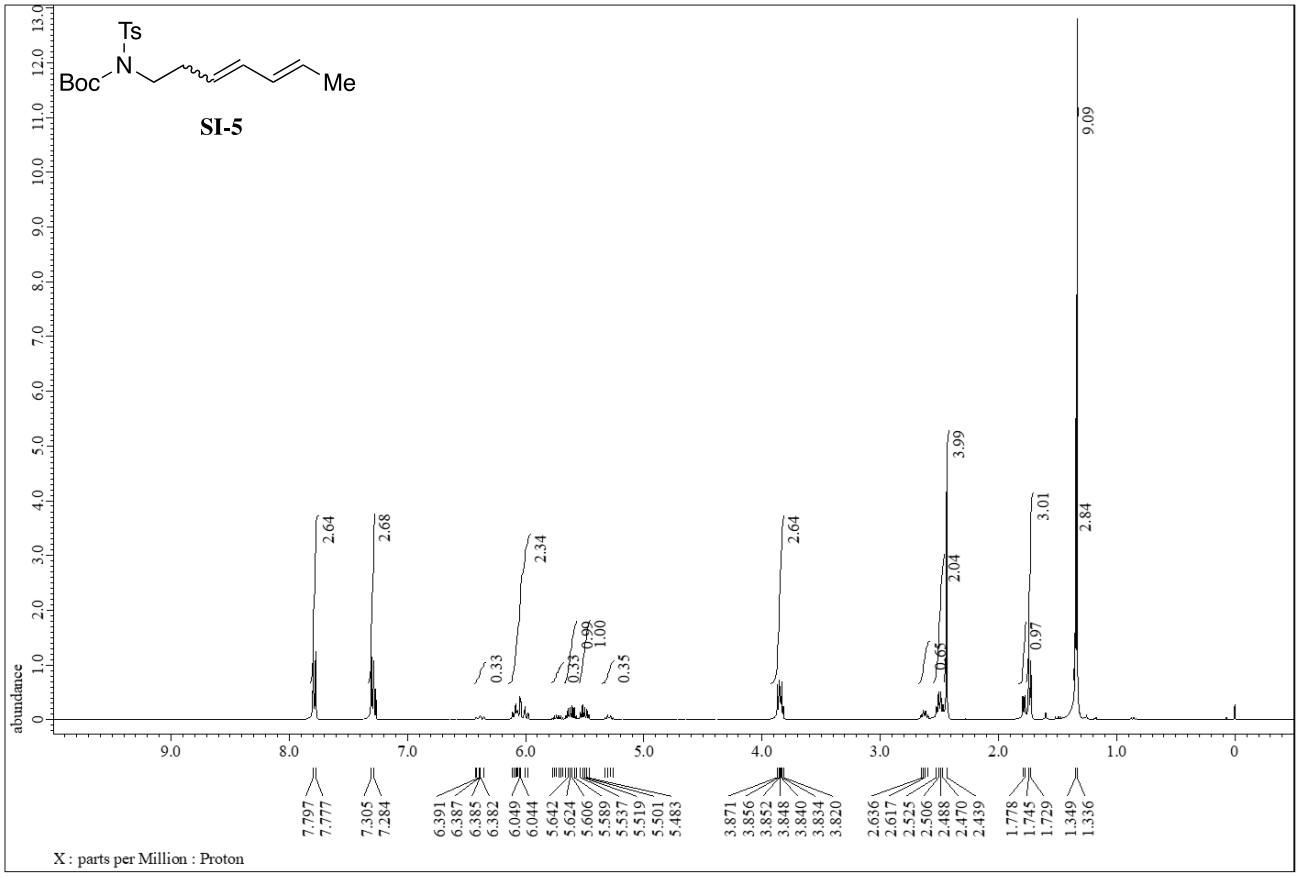

(thousandths)
X : parts per Million : Carbon13

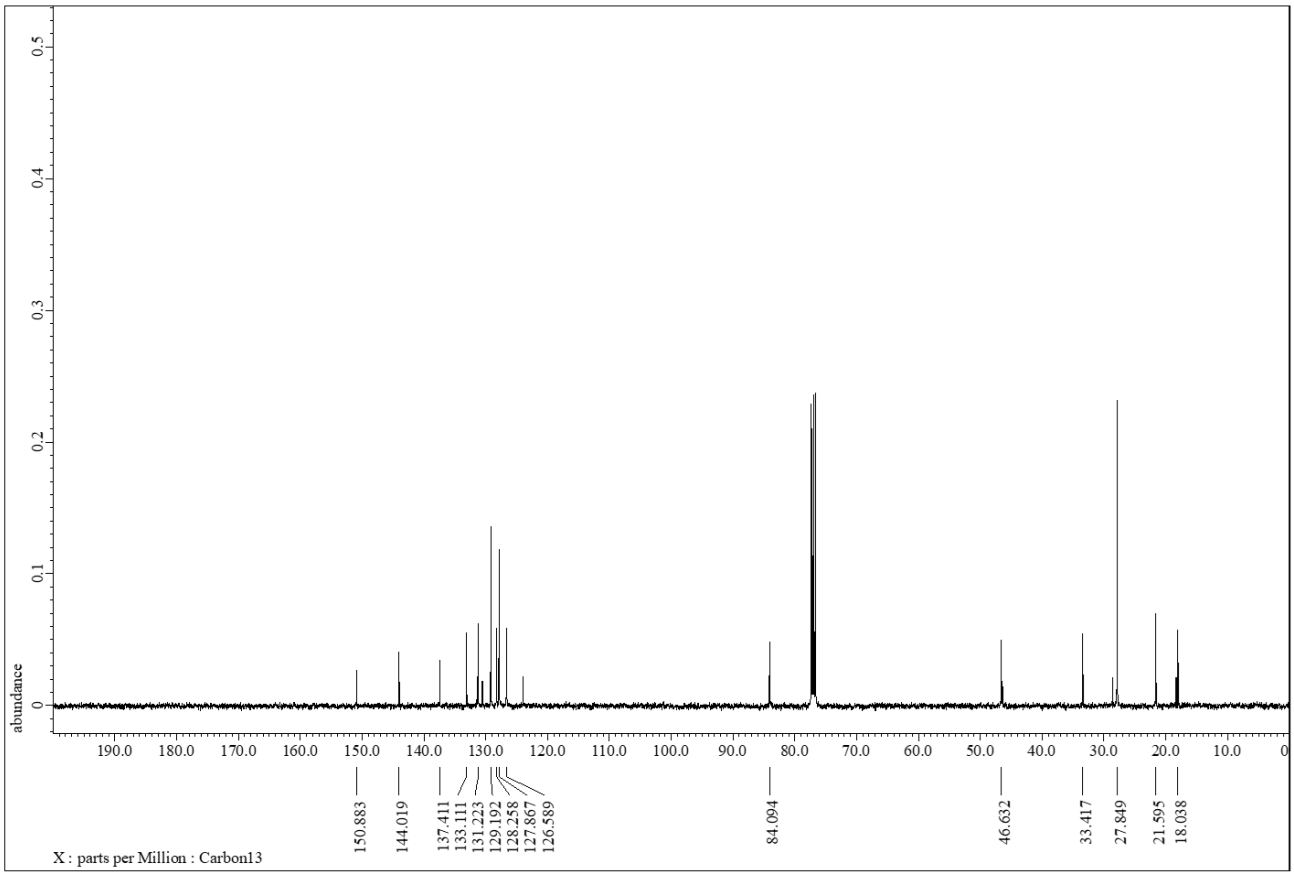

COOCH3
H3COOC
Me
SI-3
abundance
X : parts per Million : Proton

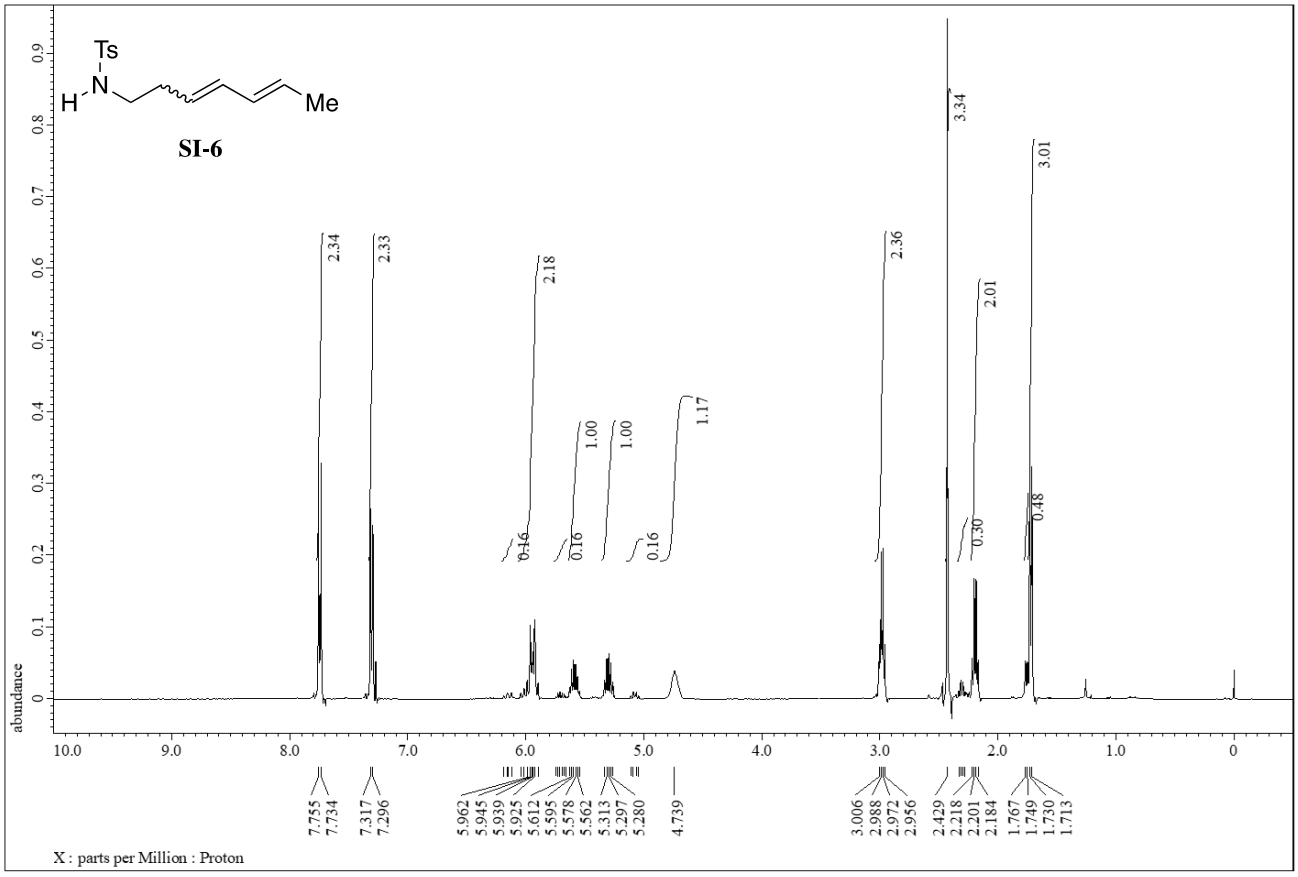

abundance
X : parts per Million : Carbon13

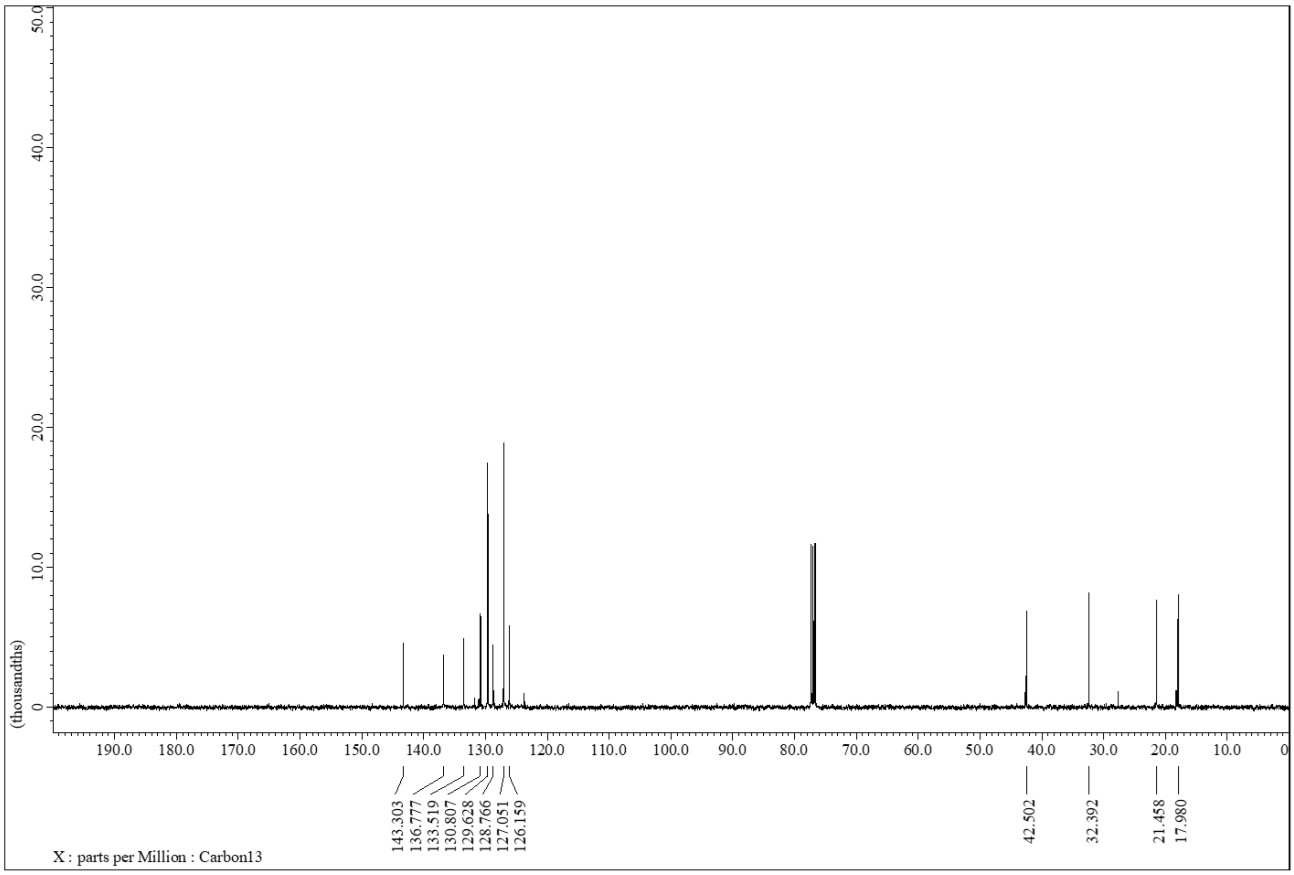

COOCH3
H3COOC
Ph
SI-4
abundance
X : parts per Million : Proton


(thousandths)
X : parts per Million : Carbon13


Ts
N
Boc
Me
SI-5
abundance
X : parts per Million : Proton


abundance
X : parts per Million : Carbon13


Ts
N
H
Me
SI-6
abundance
X : parts per Million : Proton


(thousandths)
X : parts per Million : Carbon13