Supporting Information

Synthesis of thieno[2,3-*b*]quinolone and selenopheno[2,3-*b*]quinolone derivatives *via* iodocyclization reaction and DFT mechanistic study

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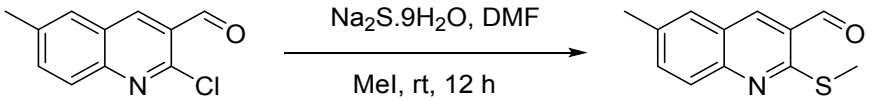
List of the Content:

Experimental: General

All solvents and reagents were purchased from the suppliers and used without further purification. IR spectra were recorded on a JASCO FT/IR-460 Plus spectrophotometer. Reactions were monitored by TLC on silica plates using UV-light or Iodine chamber for visualization. Evaporation and condensation were carried out *in vacuo*. NMR spectra were recorded with JEOL JNM-ECS 400 spectrometers with tetramethylsilane as an internal standard. Chemical shifts δ and coupling constants J are given in ppm (parts per million) and Hz (hertz) respectively. The following abbreviations were used as follows: s: singlet, d: doublet, t: triplet, m: multiplet. All known compounds data are in consistent with the given literature reports. Scale up reactions also performed as per the given general procedure without any deviation. Melting points were measured by a Yanaco micromelting point apparatus.

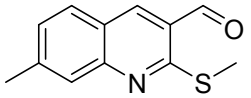
General procedure for Synthesis of 2-mercapto-quinoline-3-carbaldehyde 1a-1d:



1a

A mixture of $Na_2S.9H_2O$ (569 mg, 7.29 mmol) and 2-chloro-6-methylquinoline-3-carbaldehyde[16] (prepared according to literature reports) (1 g, 4.86 mmol) in DMF (10 mL) was stirred for 6 h room temp. Then MeI (0.303 mL, 4.86 mmol) was added. After completion of the reaction, the resulting mixture was washed with water (20 mL) and extracted with ethyl acetate (20X2), further washed organic layer with brine. Purification was performed with column chromatography using hexane / ethyl acetate (95:5) as eluent to afford **1a** 0.807 g. Yield: 76%; Melting point: 64-67^{0}C; IR (neat): 2919, 1728, 1623, 1682, 1587, 1547, 1334, 1039, 1095, 178, 825, 622, 558 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 10.29 (s, 1H), 8.34 (s, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.61 (d, *J* = 8.1 Hz, 2H), 2.70 (s, 3H), 2.52 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 190.23, 158.64, 148.38, 141.86, 136.14, 135.30, 128.07, 127.88, 127.28, 124.55, 21.50, 13.09; HRMS (ESI): m/z = 218.0640 calcd. For $C_{12}H_{12}NOS$, found 218.0612 $[M+H]^+$.

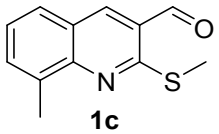
7-Methyl-2-(methylthio)quinoline-3-carbaldehyde (1b)



1b

Yield: 77%; Melting point: 88-90 ^{0}C; IR (neat): 2919, 1677, 1622, 1591, 1546, 1390, 1360, 1332, 1141, 1068, 959, 928, 800, 770, 740, 578, 469 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 10.26 (s, 1H), 8.36 (s, 1H), 7.73 (t, *J* = 8.5 Hz, 2H), 7.32 (d, *J* = 9.9 Hz, 1H), 2.69 (s, 3H), 2.56 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 190.07, 159.71, 149.87, 144.19, 142.20, 128.94, 128.43, 127.41, 126.68, 122.54, 22.29, 13.08; HRMS (ESI): m/z = 218.0640 calcd. For $C_{12}H_{12}NOS$, found 218.0632 $[M+H]^+$.

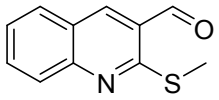
8-Methyl-2-(methylthio)quinoline-3-carbaldehyde (1c)



1c

Yield: 71%; Melting point: 86-88 ^{0}C; IR (neat): 2850, 1681, 1647, 1611, 1566, 1392, 1368, 1100, 1028, 775, 761, 524 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 10.28 (s, 1H), 8.39 (s, 1H), 7.69 (d, *J* = 8.1 Hz, 1H), 7.64 (d, *J* = 7.2 Hz, 1H), 7.39 (t, *J* = 7.4 Hz, 1H), 2.74 (s, 3H), 2.70 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 190.31, 158.38, 148.35, 143.06, 136.51, 133.21, 127.10, 126.97, 125.95, 124.33, 17.83, 13.28; HRMS (ESI): m/z = 218.0640 calcd. For $C_{12}H_{12}NOS$, found 218.0611 $[M+H]^+$.

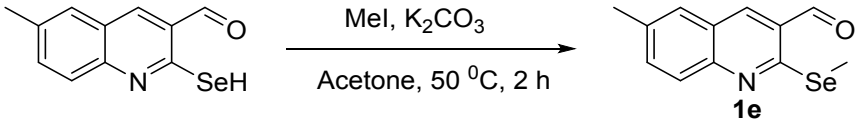
2-(Methylthio)quinoline-3-carbaldehyde (1d)



1d

Yield: 79%; Melting point: 91-93 ^{0}C; IR (neat): 2924, 1682, 1617, 1588, 1551, 1387, 1135, 1061, 804, 778, 769, 744, 479 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 10.28 (s, 1H), 8.41 (s, 1H), 7.96 (d, *J* = 8.5 Hz, 1H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.78 (t, *J* = 7.9 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 1H), 2.70 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 190.08, 159.74, 149.72, 142.42, 133.06, 129.30, 128.20, 127.32, 126.22, 124.55, 13.11; HRMS (ESI): m/z = 204.0483 calcd. For $C_{11}H_{10}NOS$, found 204.0462 $[M+H]^+$.

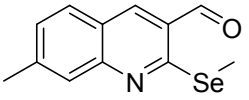
General procedure for synthesis of 6-methyl-2-(methylthio)quinoline-3-carbaldehyde 1e-1h:



1e

To a stirred solution of 2-hydroseleno-6-methylquinoline-3-carbaldehyde[16] (prepared according to literature reports) (500 mg, 2.0 mmol), MeI (0.249 mL, 4.0 mmol) and K_2CO_3 (0.552 g, 4.0 mmol) in dry acetone (15 mL) was heated at 50 ^{0}C for 2 h. The reaction mixture was turned green, after completion of reaction (monitored by TLC); the mixture was filtered and washed with acetone (15 mL). Solvent was evaporated under reduced pressure to afford a crude residue. The crude was purified by column chromatography using hexanes/ethyl acetate (95:5) as eluent to give **1e** 0.337 mg. Yield: 64%; Melting point: 56-58 ^{0}C; IR (neat): 2925, 1682, 1623, 1580, 1552, 1489, 1392, 1363, 1334, 1175, 1137, 1038, 820, 780, 746, 735, 649, 551, 481 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 10.20 (s, 1H), 8.31 (s, 1H), 7.91 (d, *J* = 8.5 Hz, 1H), 7.64 (d, *J* = 8.5 Hz, 2H), 2.54 (s, 3H), 2.53 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 191.12, 155.83, 148.90, 143.59, 136.40, 135.43, 128.77, 128.15, 127.92, 124.74, 21.56, 5.46; HRMS (ESI): m/z = 266.0084 calcd. For $C_{12}H_{12}NOSe$, found 266.0054 $[M+H]^+$.

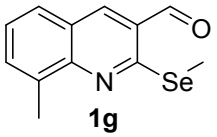
7-Methyl-2-(methylselanyl)quinoline-3-carbaldehyde (1f)



1f

Yield: 66%; Melting point: 76-78 ^{0}C; IR (neat): 2924, 1672, 1620, 1547, 1489, 1332, 1178, 1139, 1042, 1032, 1006, 878, 793, 733, 675, 571, 475 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 10.11 (s, 1H), 8.26 (s, 1H), 7.74 (s, 1H), 7.70 (d, *J* = 8.5 Hz, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 2.55 (s, 3H), 2.52 (d, *J* = 6.7 Hz, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 190.91, 157.01, 150.22, 144.30, 143.82, 128.77, 128.62, 128.11, 127.61, 122.66, 22.31, 5.46; HRMS (ESI): m/z = 266.0084 calcd. For $C_{12}H_{12}NOSe$, found 266.0056 $[M+H]^+$.

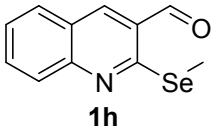
8-Methyl-2-(methylselanyl)quinoline-3-carbaldehyde (1g)



1g

Yield: 58%; Melting point: 96-98 ^{0}C; IR (neat): 2360, 2348, 2341, 1688, 1612, 1567, 1390, 1216, 1020, 756, 670, 649 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 10.20 (s, 1H), 8.35 (s, 1H), 7.70 (d, *J* = 8.2 Hz, 1H), 7.65 (d, *J* = 6.9 Hz, 1H), 7.42 (t, *J* = 7.6 Hz, 1H), 2.76 (s, 3H), 2.54 (t, *J* = 6.9 Hz, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 191.12, 155.82, 148.78, 144.49, 136.82, 133.31, 128.53, 126.99, 126.18, 124.53, 17.82, 5.66; HRMS (ESI): m/z = 266.0084 calcd. For $C_{12}H_{12}NOSe$, found 266.0055 $[M+H]^+$.

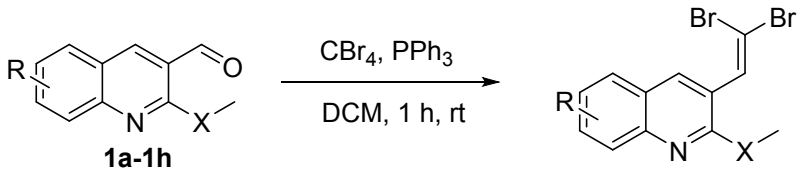
2-(Methylselanyl)quinoline-3-carbaldehyde (1h)



1h

Yield: 62%; Melting point: 69-72 ^{0}C; IR (neat): 2919, 1834, 1672, 1615, 1582, 1383, 1327, 1181, 1130, 1040, 974, 955, 921, 766, 740, 601, 478 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 10.22 (s, 1H), 8.41 (s, 1H), 8.01 (d, *J* = 9.0 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.79-7.83 (m, 1H), 7.54 (t, *J* = 7.0 Hz, 1H), 2.55 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 191.02, 157.15, 150.16, 144.16, 133.19, 129.18, 128.80, 128.49, 126.44, 124.71, 5.58; HRMS (ESI): m/z = 251.9928 calcd. For $C_{11}H_{10}NOSe$, found 251.9902 $[M+H]^+$.

General procedure for the synthesis of dibromo compounds

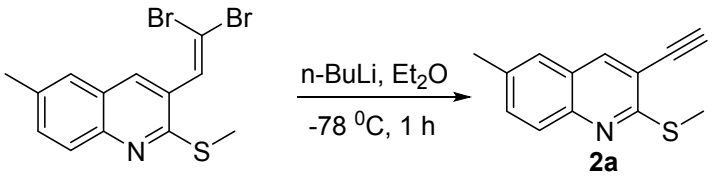


1a-1h

X = S, Se

To a stirred solution of **1a** (500 mg, 3.5 mmol) and carbon tetrabromide (1.53 g, 7 mmol, 2 equiv) in anhydrous dichloromethane (10 mL) was added triphenylphosphine (2.41 g, 14 mmol, 4 equiv) in portions over a period of 20 min at 0 °C. The reaction mixture was turned brown that was allowed to stir at 0 °C temperature for 2 h. After completion of reaction (monitored by TLC), reaction mixture was quenched with water (15 mL). The reaction mixture was extracted with dichloromethane (2 x 20 mL); organic layer was washed with brine (10 mL); dried over anhydrous Na_2SO_4; solvent was evaporated under reduced pressure to afford a crude residue. After purification by column chromatography, the isolated dibromo olefins were used for next step.[17]

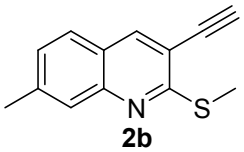
General procedure for the synthesis of 3-ethynyl-6-methyl-2-(methylthio)quinoline 2a-2g:



2a

3-(2,2-Dibromovinyl)-6-methyl-2-(methylthio)quinoline[17] (0.250 g, 0.67 mmol, 1 equiv.) was dissolved in dry ether (6 mL) and cooled to -78 °C under an atmospheric nitrogen; n-BuLi (1.64M in hexane, 1.1 mL, 1.68 mmol, 2.5 equiv.) was added drop wise over 10 minutes and the solution was stirred for a further 1 h then for 30 min at room temperature. The reaction was quenched with water (20 mL), and extracted with ether (2 × 10 mL). The organic layers was combined, dried over sodium sulfate and concentrated in vacuo; purified by column chromatography using hexanes/ethyl acetate (98:2) as eluent to afford **2a** 0.096 g; yellow sticky compound. Yield: 67%; IR (KBr): 2361, 2341, 1675, 1616, 1585, 1555, 1387, 1363, 1336, 1317, 1216, 1137, 1048, 955, 915, 751, 668, 601 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.83 (d, *J* = 8.2 Hz, 1H), 7.48 (d, *J* = 8.2 Hz, 1H), 7.43 (s, 1H), 3.54 (s, 1H), 2.69 (s, 3H), 2.49 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 159.53, 145.93, 139.18, 135.58, 132.79, 127.72, 126.42, 124.82, 115.14, 84.95, 79.49, 21.54, 13.37; HRMS (ESI): m/z = 214.0690 calcd. For $C_{13}H_{12}NS$, found 214.0660 $[M+H]^+$.

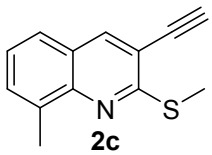
3-Ethynyl-7-methyl-2-(methylthio)quinoline (2b)



2b

Yield: 69%; Melting point: 93-96 ^{0}C; IR (neat): 3196, 2095, 1900, 1621, 1582, 1488, 1390, 1363, 1137, 1052, 1037, 871, 796, 726, 618, 486 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.04 (s, 1H), 7.73 (s, 1H), 7.56 (d, *J* = 8.1 Hz, 1H), 7.25 (t, *J* = 3.4 Hz, 1H), 3.53 (s, 1H), 2.68 (s, 3H), 2.53 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.56, 147.49, 141.20, 139.39, 127.91, 127.29, 127.13, 122.83, 114.34, 84.76, 79.49, 22.01, 13.33; HRMS (ESI): m/z = 214.0690 calcd. For $C_{13}H_{12}NS$, found 214.0663 $[M+H]^+$.

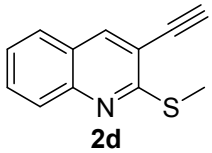
3-Ethynyl-8-methyl-2-(methylthio)quinoline (2c)



2c

Yield: 72%; Melting point: 73-76 ^{0}C; IR (neat): 3020, 2361, 2641, 1616, 1556, 1216, 1137, 1051, 756, 670, 662 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.52 (t, *J* = 6.2 Hz, 2H), 7.32 (t, *J* = 7.6 Hz, 1H), 3.55 (s, 1H), 2.74 (s, 3H), 2.70 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 159.35, 146.00, 139.96, 136.16, 130.87, 125.50, 125.37, 124.63, 114.85, 84.94, 79.44, 17.78, 13.50; HRMS (ESI): m/z = 214.0690 calcd. For $C_{13}H_{12}NS$, found 214.0663 $[M+H]^+$.

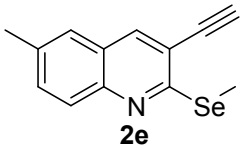
3-Ethynyl-2-(methylthio)quinoline (2d)



2d

Yield: 75%; Melting point: 69-71 ^{0}C; IR (neat): 2928, 1676, 1555, 1585, 1387, 1216, 1137, 1048, 915, 755, 668, 601 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.93 (d, *J* = 8.5 Hz, 1H), 7.63-7.69 (m, 2H), 7.43 (t, *J* = 7.6 Hz, 1H), 3.55 (s, 1H), 2.70 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.68, 147.29, 139.64, 130.61, 128.03, 127.50, 125.76, 124.83, 115.28, 85.12, 79.30, 13.39; HRMS (ESI): m/z = 200.0534 calcd. For $C_{12}H_{10}NS$, found 200.0504 $[M+H]^+$.

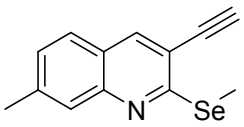
3-Ethynyl-6-methyl-2-(methylselanyl)quinoline (2e)



2e

Yield: 65%; Melting point: 54-56 ^{0}C; IR (neat): 3299, 2931, 1580, 1555, 1491, 1390, 1335, 1261, 1216, 1172, 1035, 918, 832, 758, 691, 665, 573 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.77 (d, *J* = 8.5 Hz, 1H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.37 (s, 1H), 3.45 (s, 1H), 2.51 (s, 3H), 2.41 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 156.75, 146.51, 138.53, 135.85, 132.74, 127.90, 126.47, 125.26, 117.45, 84.54, 80.10, 21.56, 6.07; HRMS (ESI): m/z = 262.0135 calcd. For $C_{13}H_{12}NSe$, found 262.0109 $[M+H]^+$.

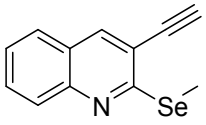
3-Ethynyl-7-methyl-2-(methylselanyl)quinoline (2f)



2f

Yield: 66%; Melting point: 75-78 ^{0}C; IR (neat): 3202, 2361, 2342, 1623, 1336, 1216, 1033, 756, 670, 484 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.74 (s, 1H), 7.57 (d, *J* = 8.5 Hz, 1H), 7.28 (d, *J* = 8.1 Hz, 1H), 3.51 (s, 1H), 2.58 (t, *J* = 6.3 Hz, 3H), 2.53 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 157.93, 148.01, 141.17, 138.76, 128.17, 127.44, 127.22, 123.28, 116.66, 84.37, 80.10, 22.00, 6.07; HRMS (ESI): m/z = 262.0135 calcd. For $C_{13}H_{12}NSe$, found 262.0142 $[M+H]^+$.

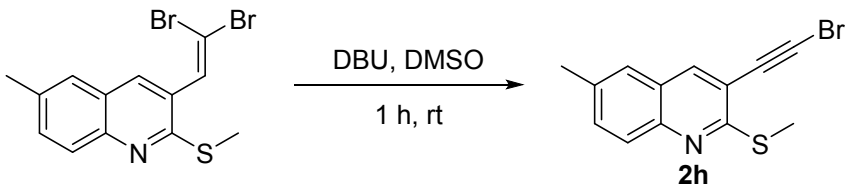
3-Ethynyl-2-(methylselanyl)quinoline (2g)



2g

Yield: 71%; Sticky; IR (KBr): 3302, 2934, 2341, 1617, 1583, 1555, 1360, 1216, 1134, 1031, 915, 753, 669, 612 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.95 (d, *J* = 9.2 Hz, 1H), 7.63-7.69 (m, 2H), 7.45 (t, *J* = 7.6 Hz, 1H), 3.53 (s, 1H), 2.60 (d, *J* = 6.0 Hz, 3H); ^{13}C-NMR (101 MHz, $CDCl_3$) δ 158.11, 147.83, 138.99, 130.55, 128.22, 127.58, 126.00, 125.28, 117.60, 84.72, 79.94, 6.16; HRMS (ESI): m/z = 247.9978 calcd. For $C_{12}H_{10}NSe$, found 247.9959 $[M+H]^+$.

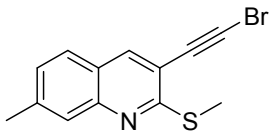
General procedure for the synthesis of 3-(bromoethynyl)-6-methyl-2-(methylthio)quinoline 2h-2n:



2h

3-(2,2-Dibromovinyl)-6-methyl-2-(methylthio)quinoline[17] (100 mg, 1 mmol, 1 equiv.) in DMSO (2 mL) was added DBU (111 mg, 2.0 mmol, 2 equiv.) drop wise over a period of 5 min at 15-20 °C temperature. The reaction mixture was allowed to stir at the same temperature for 30 min. after completion; reaction mixture was quenched by drop wise addition of 5N aqueous HCl (10 mL) over a period of 10 min then continued stirring for 5 min. The reaction mixture was extracted with dichloromethane (2 x 10 mL); organic layer was washed with water (10 mL). The organic layers was combined, dried over sodium sulfate and concentrated in vacuo; purified by column chromatography using hexanes/ethyl acetate (97:3) as eluent to afford **2h** 60 mg; pale yellow sticky liquid. Yield: 77%; IR (KBr): 2928, 1585, 1559, 1492, 1338, 1215, 1140, 1071, 920, 826, 759, 669, 581 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1H), 7.80 (d, *J* = 8.5 Hz, 1H), 7.46 (d, *J* = 8.5 Hz, 1H), 7.39 (s, 1H), 2.67 (s, 3H), 2.47 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 159.76, 145.75, 138.81, 135.58, 132.70, 127.71, 126.36, 124.82, 115.83, 76.20, 57.90, 21.51, 13.31; HRMS (ESI): m/z = 291.9801 calcd. For $C_{13}H_{11}NSBr$, found 291.9801 $[M+H]^+$.

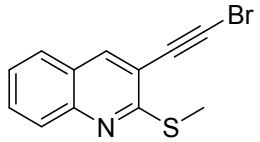
3-(Bromoethynyl)-7-methyl-2-(methylthio)quinoline (2i)



2i

Yield: 86%; Melting point: 88-91 ^{0}C; IR (neat): 2924, 2368, 2190, 1587, 1622, 1492, 1390, 1338, 1143, 1067, 912, 880, 802, 621 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.73 (s, 1H), 7.57 (d, J = 8.1 Hz, 1H), 7.29-7.27 (1H), 2.68 (s, 3H), 2.53 (s, 3H); HRMS (ESI): m/z = 291.9796 calcd. For $C_{13}H_{11}NSBr$, found 291.9796 $[M+H]^+$.

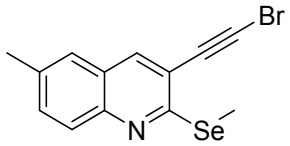
3-(Bromoethynyl)-2-(methylthio)quinoline (2j)



2j

Yield: 84%; Melting point: 46-48 ^{0}C; IR (neat): 2924, 2191, 1614, 1584, 1552, 1485, 1387, 1362, 1336, 1135, 1064, 955, 778, 751, 601, 480 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.00 (s, 1H), 7.90 (d, *J* = 9.0 Hz, 1H), 7.60-7.64 (m, 2H), 7.39 (t, *J* = 7.6 Hz, 1H), 2.67 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.89, 147.10, 139.29, 130.55, 128.01, 127.46, 125.77, 124.83, 115.94, 85.16, 76.85, 58.20, 13.38; HRMS (ESI): m/z = 277.9639 calcd. For $C_{12}H_9NSBr$, found 277.9649 $[M+H]^+$.

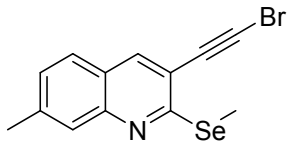
3-(Bromoethynyl)-6-methyl-2-(methylselanyl)quinoline (2k)



2k

Yield: 81%; Sticky; IR (KBr): 2921, 2190, 1771, 1581, 1551, 1490, 1389, 1335, 1038, 915, 820, 725, 568, 479 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.88 (s, 1H), 7.81 (d, *J* = 8.5 Hz, 1H), 7.45 (d, *J* = 8.5 Hz, 1H), 7.39 (s, 1H), 2.56 (s, 3H), 2.46 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 156.99, 146.33, 138.20, 135.87, 132.68, 127.88, 126.44, 125.26, 118.10, 57.66, 21.56, 6.05; HRMS (ESI): m/z = 339.9240 calcd. For $C_{13}H_{11}NBrSe$, found 339.9217 $[M+H]^+$.

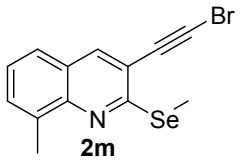
3-(Bromoethynyl)-7-methyl-2-(methylselanyl)quinoline (2l)



2l

Yield: 77%; Sticky; IR (KBr): 3016, 1710, 1421, 1363, 1223, 757, 531 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.71 (s, 1H), 7.52 (d, *J* = 8.1 Hz, 1H), 7.25 (t, *J* = 4.3 Hz, 1H), 2.57 (d, *J* = 6.3 Hz, 3H), 2.51 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 158.16, 147.81, 141.14, 138.44, 128.18, 127.43, 127.20, 123.27, 117.29, 84.41, 57.42, 22.04, 6.07; HRMS (ESI): m/z = 339.9240 calcd. For $C_{13}H_{11}NSeBr$, found 339.9228 $[M+H]^+$.

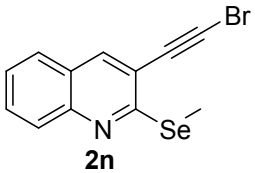
3-(bromoethynyl)-8-methyl-2-(methylselanyl)quinoline (2m)



2m

Yield: 71%; Sticky; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 2.3 Hz, 1H), 7.49-7.52 (m, 2H), 7.34 (t, *J* = 7.6 Hz, 1H), 2.75 (s, 3H), 2.60 (t, *J* = 3.0 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 157.02, 146.36, 139.00, 136.31, 130.82, 125.78, 125.45, 125.10, 117.88, 77.43, 77.12, 76.79, 57.61, 17.72, 6.17.

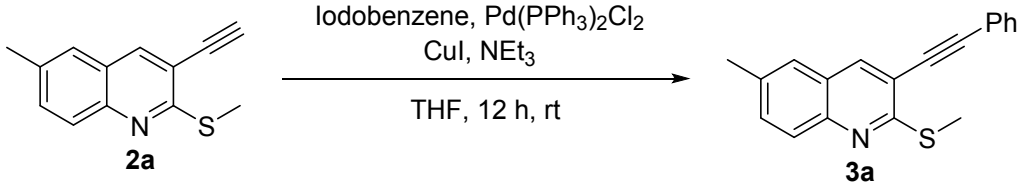
3-(Bromoethynyl)-2-(methylselanyl)quinoline (2n)



2n

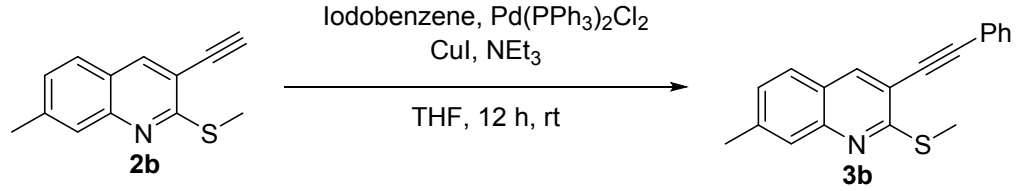
Yield: 75%; Sticky; IR (KBr): 2619, 1615, 1552, 1441, 1331, 1131, 915, 751 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.93 (d, *J* = 8.5 Hz, 1H), 7.62-7.67 (m, 2H), 7.43 (t, *J* = 7.0 Hz, 1H), 2.58 (t, *J* = 6.1 Hz, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ 158.35, 147.65, 138.67, 130.52, 128.19, 127.56, 126.03, 125.27, 118.25, 57.93, 6.15; HRMS (ESI): m/z = 325.9084 calcd. For $C_{12}H_9NSeBr$, found 325.9077 $[M+H]^+$.

General procedure for the synthesis of 6-methyl-2-(methylthio)-3-(phenylethynyl)quinoline 3a-3g:



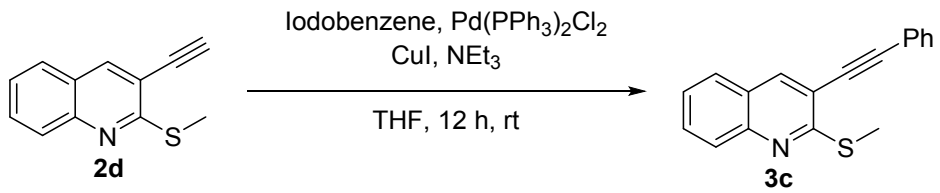
To solution of 3-ethynyl-6-methyl-2-(methylthio)quinoline **2a** (30 mg, 0.140 mmol) dissolved in triethylamine (3 ml); Iodobenzene (57.39 mg, 0.0.281 mmol, 2 equiv.), $Pd(PPh_3)_2Cl_2$ (9.9 mg, 0.014 mmol, 0.1 equiv.), copper(I) iodide (2.68 mg, 0.014 mmol, 0.1 equiv) were added under nitrogen atmosphere. The mixture was stirred at room temperature for 12 h. After completion, the mixture was concentrated in vacuo to remove triethylamine. The crude product was dissolved in dichloromethane and extracted with aqueous ammonium chloride solution. The crude product was isolated by evaporating the solvent and purified by column chromatography using hexane/ethyl acetate (96:4) as eluent to afford **3a** 31 mg; yellow syrup. Yield: 76%; IR (KBr): 2926, 2158, 1676, 1616, 1584, 1555, 1486, 1317, 1174, 1028, 956, 914, 752, 667, 601, 583 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.02 (s, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.61-7.63 (m, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.38 (t, *J* = 2.7 Hz, 3H), 2.70 (s, 3H), 2.50 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 159.81, 145.72, 137.50, 135.44, 132.40, 131.76, 128.88, 128.52, 127.71, 126.45, 125.10, 122.83, 116.40, 97.05, 85.26, 21.54, 13.38; HRMS (ESI): m/z = 290.1003 calcd. For $C_{19}H_{16}NS$, found 290.0991 $[M+H]^+$.

7-Methyl-2-(methylthio)-3-(phenylethynyl)quinoline (3b)



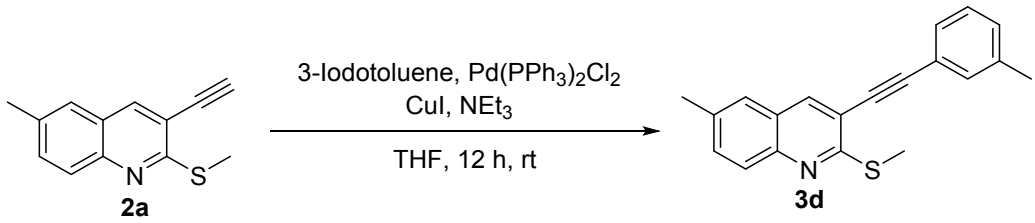
Yield: 79%; Sticky; IR (KBr): 2927, 2378, 2158, 1676, 1616, 1585, 1363, 1317, 1174, 1048, 956, 860, 693, 667, 583, 485 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.75 (s, 1H), 7.59-7.63 (m, 3H), 7.38 (t, *J* = 2.7 Hz, 3H), 7.28 (s, 1H), 2.71 (s, 3H), 2.54 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.83, 147.27, 140.81, 137.78, 131.72, 128.83, 128.51, 127.81, 127.29, 127.18, 123.11, 122.87, 115.58, 96.88, 85.25, 22.01, 13.39; HRMS (ESI): m/z = 290.1003 calcd. For $C_{19}H_{16}NS$, found 290.0974 $[M+H]^+$.

2-(Methylthio)-3-(phenylethynyl)quinoline (3c)



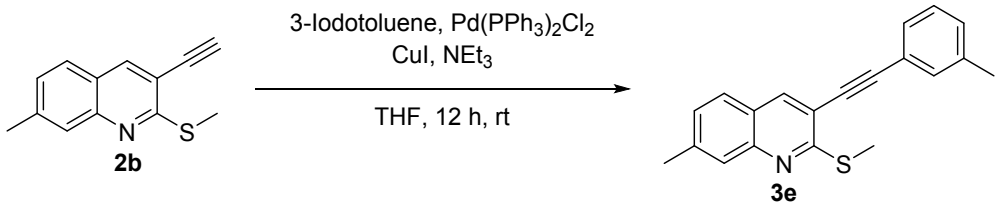
Yield: 87%; Melting point: 54-56 ^{0}C; IR (KBr): 2927, 2361, 2642, 1615, 1585, 1555, 1486, 1363, 1335, 1317, 1137, 955, 753, 670, 662 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.95 (d, *J* = 9.0 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.62-7.67 (m, 3H), 7.44 (d, *J* = 6.7 Hz, 1H), 7.38-7.41 (m, 3H), 2.72 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.93, 147.07, 137.96, 131.77, 130.24, 128.95, 128.54, 128.00, 127.52, 125.67, 125.12, 122.76, 116.53, 97.22, 85.08, 13.43; HRMS (ESI): m/z = 276.0847 calcd. For $C_{18}H_{14}NS$, found 276.0823 $[M+H]^+$.

6-Methyl-2-(methylthio)-3-(m-tolylethynyl)quinoline (3d)



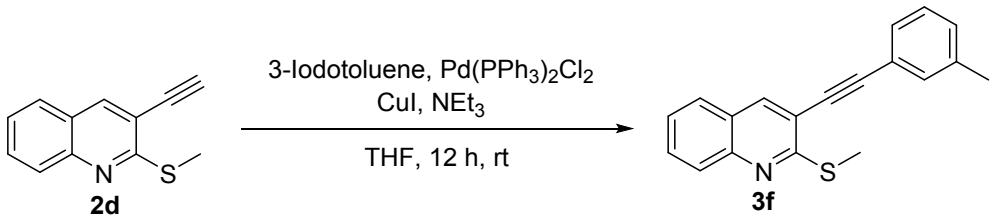
Yield: 80%; Melting point: 107-109 ^{0}C; IR (neat): 2063, 1631, 1348, 1362, 1058, 821, 782, 689, 540 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.42-7.48 (m, 4H), 7.28 (d, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 7.6 Hz, 1H), 2.70 (s, 3H), 2.49 (s, 3H), 2.38 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 159.83, 145.68, 138.23, 137.42, 135.41, 132.35, 132.28, 129.80, 128.84, 128.41, 127.70, 126.44, 125.12, 122.60, 116.50, 97.29, 84.91, 21.54, 21.35, 13.39; HRMS (ESI): m/z = 304.1160 calcd. For $C_{20}H_{18}NS$, found 304.1131 $[M+H]^+$.

7-Methyl-2-(methylthio)-3-(m-tolylethynyl)quinoline (3e)



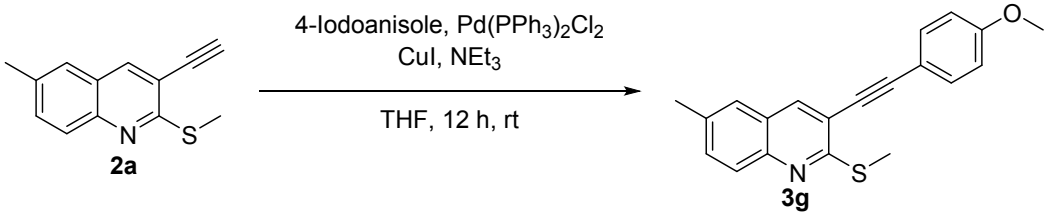
Yield: 75%; Sticky; IR (KBr): 2927, 2159, 1676, 1585, 1363, 1336, 1317, 1174, 1048, 915, 668, 601, 583, 485 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.75 (s, 1H), 7.59 (d, *J* = 8.5 Hz, 1H), 7.41-7.45 (m, 2H), 7.28 (d, *J* = 7.2 Hz, 1H), 7.25 (s, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 2.70 (s, 3H), 2.54 (s, 3H), 2.38 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.85, 147.23, 140.75, 138.21, 137.70, 132.26, 129.76, 128.81, 128.40, 127.79, 127.28, 127.17, 123.13, 122.66, 115.68, 97.12, 84.89, 22.01, 21.35, 13.39; HRMS (ESI): m/z = 304.1160 calcd. For $C_{20}H_{18}NS$, found 304.1142 $[M+H]^+$.

2-(Methylthio)-3-(m-tolylethynyl)quinoline (3f)



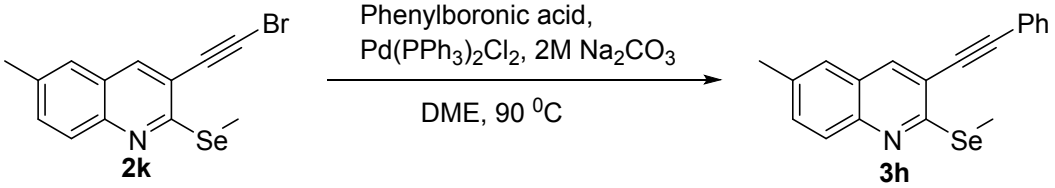
Yield: 72%; Melting point: 52-54 ^{0}C; IR (neat): 2923, 1585, 1556, 1443, 1387, 1362, 1343, 1135, 1052, 908, 777, 749, 688, 599, 493 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.70 (d, *J* = 8.1 Hz, 1H), 7.62-7.66 (m, 1H), 7.40-7.45 (m, 3H), 7.28 (d, *J* = 7.6 Hz, 1H), 7.19 (d, *J* = 7.6 Hz, 1H), 2.72 (s, 3H), 2.38 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.95, 147.04, 138.25, 137.88, 132.30, 130.19, 129.87, 128.86, 128.43, 128.00, 127.51, 125.64, 125.14, 122.54, 116.62, 97.45, 84.74, 21.35, 13.43; HRMS (ESI): m/z = 290.1003 calcd. For $C_{19}H_{16}NS$, found 290.0983 $[M+H]^+$.

3-((4-Methoxyphenyl)ethynyl)-6-methyl-2-(methylthio)quinoline (3g)



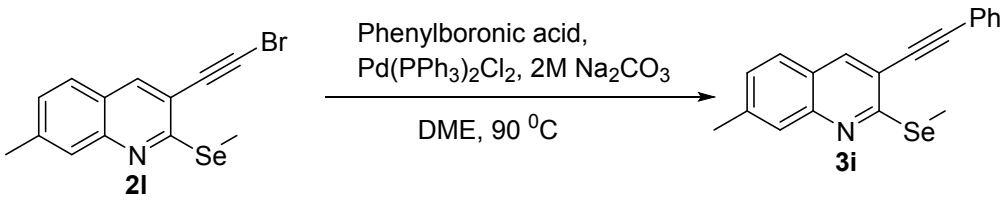
Yield: 70%; Melting point: 84-86 ^{0}C; IR (neat): 2923, 2206, 1601, 1582, 1566, 1508, 1289, 1246, 1146, 1126, 1053, 1023, 833, 819, 637, 582, 539, 526 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.99 (s, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.56 (d, *J* = 9.0 Hz, 2H), 7.45 (s, 2H), 6.91 (d, *J* = 8.5 Hz, 2H), 3.85 (s, 3H), 2.70 (s, 3H), 2.51-2.50 (3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.14, 145.55, 139.97, 137.04, 133.28, 133.18, 132.20, 127.76, 127.68, 126.53, 125.18, 116.75, 114.17, 97.24, 84.07, 55.44, 21.54, 13.39; HRMS (ESI): m/z = 320.1109 calcd. For $C_{20}H_{18}NOS$, found 320.1082 $[M+H]^+$.

General procedure for the synthesis of 6-methyl-2-(methylselanyl)-3-(phenylethynyl)quinoline 3h-3j:



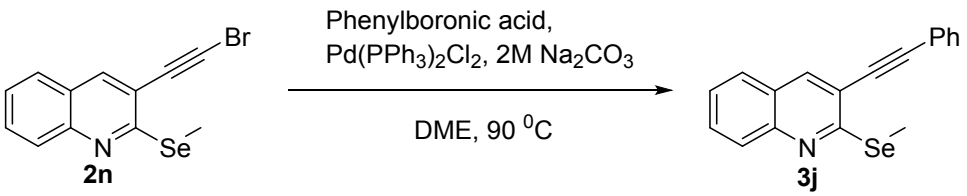
To the solution of 3-(bromoethynyl)-6-methyl-2-(methylselanyl)quinoline **2k** (100 mg, 294.9 mmol, 1 equiv.) in DME (1.5 mL) was added 2M Na_2CO_3 (1 ml) and $Pd(PPh_3)_2Cl_2$ (20.7 mg, 20.49 mmol, 0.1 equiv); the reaction mixture was allowed to stir at 90^0C for 1 h. The reaction mixture was extracted with ethyl acetate: brine (2 x 10 mL). The organic layer was dried over anhydrous sodium sulfate; the crude product was isolated by evaporating the solvent and purified by column chromatography using hexane/ ethyl acetate (98:2) as eluent to afford **3h** 69 mg; pale yellow syrup. Yield: 70%; IR (KBr): 2927, 1581, 1554, 1492, 1392, 1348, 1141, 1040, 914, 822, 755, 689, 574, 526 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.98 (s, 1H), 7.86 (d, *J* = 8.5 Hz, 1H), 7.64 (t, *J* = 3.6 Hz, 2H), 7.47 (d, *J* = 8.5 Hz, 2H), 7.38-7.39 (m, 3H), 2.60 (s, 3H), 2.49 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 157.23, 146.28, 136.87, 135.75, 132.39, 131.74, 128.96, 128.55, 127.89, 126.53, 125.56, 122.71, 118.66, 96.56, 85.96, 21.59, 6.02; HRMS (ESI): m/z = 338.0448 calcd. For $C_{19}H_{16}NSe$, found 338.0430 $[M+H]^+$.

7-Methyl-2-(methylselanyl)-3-(phenylethynyl)quinoline (3i)



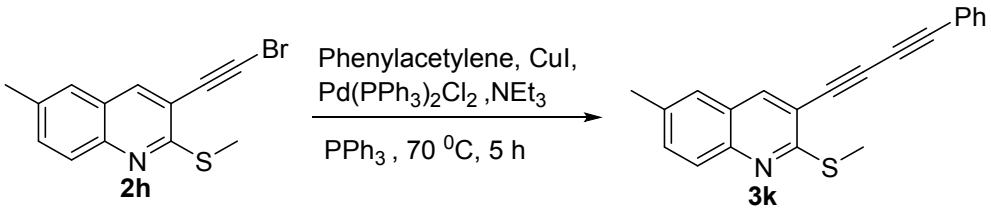
Yield: 72%; Sticky; IR (KBr): 2928, 2210, 1622, 1581, 1487, 1442, 1392, 1342, 1268, 1194, 1143, 1122, 1036, 911, 802, 755, 690, 581, 477 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.76 (s, 1H), 7.59-7.64 (m, 3H), 7.38 (dd, *J* = 5.4, 1.8 Hz, 3H), 7.28 (d, *J* = 6.7 Hz, 1H), 2.60 (t, *J* = 6.1 Hz, 3H), 2.54 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 158.41, 147.77, 140.80, 137.14, 131.71, 128.90, 128.54, 128.09, 127.44, 127.28, 123.57, 122.77, 117.86, 96.39, 85.95, 22.02, 6.04; HRMS (ESI): m/z = 338.0448 calcd. For $C_{19}H_{16}NSe$, found 338.0429 $[M+H]^+$.

2-(Methylselanyl)-3-(phenylethynyl)quinoline (3j)



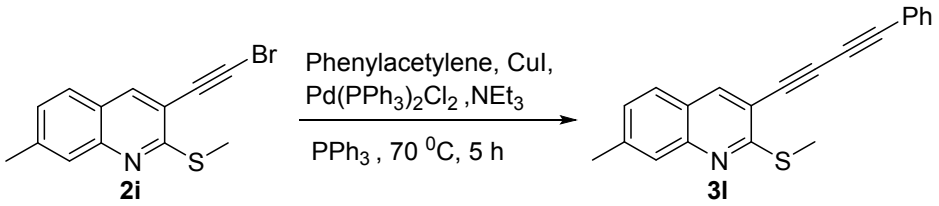
Yield: 67%; Sticky; IR (KBr): 2364, 2341, 1564, 1216, 1132, 753, 669, 662 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 7.71 (d, *J* = 8.1 Hz, 1H), 7.62-7.67 (m, 3H), 7.45 (t, *J* = 7.0 Hz, 1H), 7.39 (t, *J* = 3.4 Hz, 3H), 2.61 (t, *J* = 6.1 Hz, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 158.57, 147.58, 137.31, 131.76, 130.21, 129.01, 128.56, 128.19, 127.62, 125.92, 125.58, 122.64, 118.80, 96.73, 85.79, 6.11; HRMS (ESI): m/z = 324.0291 calcd. For $C_{18}H_{14}NSe$, found 324.0288 $[M+H]^+$.

General procedure for the synthesis of 6-methyl-2-(methylthio)-3-(phenylbuta-1,3-diyn-1-yl)quinoline 3k-3q:



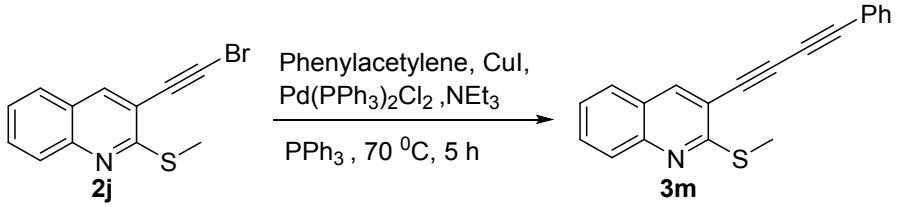
To a solution of 3-(bromoethynyl)-6-methyl-2-(methylthio)quinoline **2h** (40 mg, 0.136 mmol) dissolved in dry triethylamine (4 ml) was added phenyl acetylene (18.18 mg, 0.177 mmol, 1.3 equiv.), $Pd(PPh_3)_2Cl_2$ (7 mg, 0.6 mmol, 0.6 equiv.), triphenylphosphine (3.59 mg, 0.1 mmol, 0.1 equiv.), and copper(I) iodide (1.30 mg, 0.0068 mmol) at room temperature under nitrogen. The mixture was stirred at 70^{0}C for 8 h. After completion of reaction, the mixture concentrated in vacuo to remove triethylamine. The crude product was dissolved in dichloromethane and extracted with aqueous ammonium chloride solution. The crude product was isolated by evaporating the solvent and purified by column chromatography using hexane/ethyl acetate (97:3) as eluent to afford **3k** 28 mg; yellow solid; Yield: 65%; Melting point: 114-117 ^{0}C; IR (neat): 2918, 2206, 1841, 1678, 1579, 1557, 1488, 1399, 1360, 1309, 1140, 1083, 924, 825, 743, 678, 577, 522 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.05 (s, 1H), 7.83 (d, *J* = 8.5 Hz, 1H), 7.55-7.57 (m, 2H), 7.49 (d, *J* = 8.5 Hz, 1H), 7.45 (s, 1H), 7.34-7.40 (m, 3H), 2.70 (s, 3H), 2.50 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.16, 145.84, 139.68, 135.70, 133.03, 132.69, 129.55, 128.56, 127.74, 126.46, 124.83, 121.62, 115.13, 84.12, 81.34, 76.78, 73.73, 21.51, 13.33; HRMS (ESI): m/z = 314.1003 calcd. For $C_{21}H_{16}NS$, found 314.0978 $[M+H]^+$.

7-Methyl-2-(methylthio)-3-(phenylbuta-1,3-diyn-1-yl)quinoline (3l)



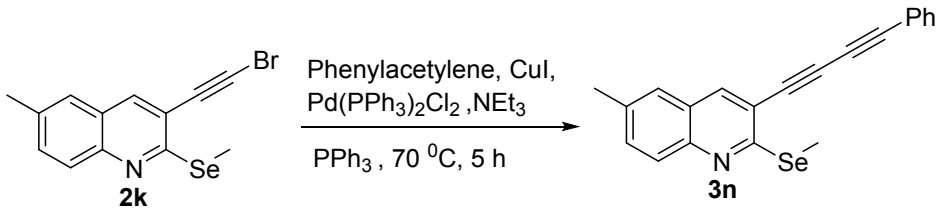
Yield: 71%; Melting point: 128-130 ^{0}C; IR (neat): 2923, 1619, 1596, 1579, 1488, 1438, 1397, 1345, 1140, 1079, 899, 875, 683, 648, 579, 524, 465 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.72 (s, 1H), 7.55 (d, *J* = 8.1 Hz, 3H), 7.36 (dd, *J* = 9.2, 7.0 Hz, 3H), 7.26 (d, *J* = 5.4 Hz, 1H), 2.69 (s, 3H), 2.53 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.19, 147.36, 141.56, 139.91, 132.68, 129.53, 128.56, 128.02, 127.33, 127.22, 122.85, 121.66, 114.27, 84.04, 81.21, 76.80, 73.81, 22.08, 13.34; HRMS (ESI): m/z = 314.1003 calcd. For $C_{21}H_{16}NS$, found 314.0976 $[M+H]^+$.

2-(Methylthio)-3-(phenylbuta-1,3-diyn-1-yl)quinoline (3m)



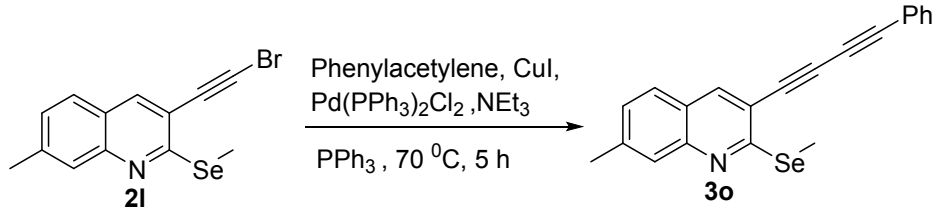
Yield: 67%; Melting point: 110-112 ^{0}C; IR (neat): 2922, 1594, 1551, 1580, 1486, 1360, 1351, 1132, 1073, 966, 951, 905, 760, 749, 687, 575, 524, 485 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.11 (s, 1H), 7.92 (d, *J* = 8.1 Hz, 1H), 7.63-7.68 (m, 2H), 7.56 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.33-7.44 (m, 4H), 2.71 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.27, 147.17, 140.13, 132.71, 130.85, 129.60, 128.58, 128.05, 127.55, 125.86, 124.83, 121.57, 115.26, 84.23, 81.52, 76.81, 73.72, 13.39; HRMS (ESI): m/z = 300.0847 calcd. For $C_{20}H_{14}NS$, found 300.0824 $[M+H]^+$.

6-Methyl-2-(methylselanyl)-3-(phenylbuta-1,3-diyn-1-yl)quinoline (3n)



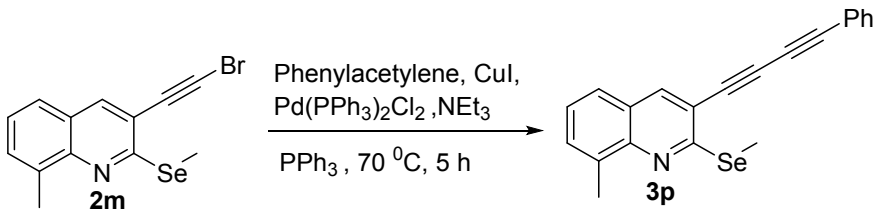
Yield: 70%; Melting point: 104-105 ^{0}C; IR (neat): 2614, 1579, 1531, 1463, 1353, 1065, 915, 823, 755, 688, 541 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 1H), 7.84 (d, *J* = 8.5 Hz, 1H), 7.57 (d, *J* = 7.6 Hz, 2H), 7.31-7.40 (m, 5H), 2.60 (s, 3H), 2.49 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 157.29, 146.41, 139.14, 135.98, 133.00, 132.71, 129.59, 128.57, 127.93, 126.52, 125.27, 121.56, 117.45, 84.10, 80.96, 76.79, 73.71, 21.55, 6.09; HRMS (ESI): m/z = 362.0448 calcd. For $C_{21}H_{16}NSe$, found 362.0439 $[M+H]^+$.

7-Methyl-2-(methylselanyl)-3-(phenylbuta-1,3-diyn-1-yl)quinoline (3o)



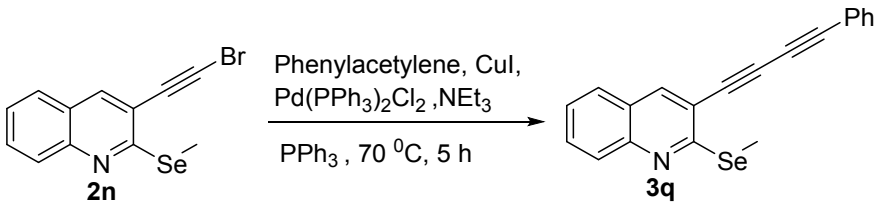
Yield: 73%; Melting point: 143-145 ^{0}C; IR (neat): 2929, 1958, 1870, 1796, 1589, 1586, 1438, 1264, 1141, 1063, 899, 793, 748, 683, 578, 524, 465 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.03 (s, 1H), 7.74 (s, 1H), 7.57 (dt, *J* = 7.9, 2.0 Hz, 3H), 7.37 (dd, *J* = 9.2, 7.0 Hz, 3H), 7.29 (d, *J* = 9.9 Hz, 1H), 2.58-2.60 (m, 3H), 2.54 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 158.49, 147.89, 141.54, 139.38, 132.69, 129.56, 128.56, 128.28, 127.49, 127.30, 123.30, 121.61, 116.63, 84.02, 80.83, 76.79, 73.76, 22.06, 6.09; HRMS (ESI): m/z = 362.0448 calcd. For $C_{21}H_{16}NSe$, found 362.0426 $[M+H]^+$.

8-Methyl-2-(methylselanyl)-3-(phenylbuta-1,3-diyn-1-yl)quinoline (3p)



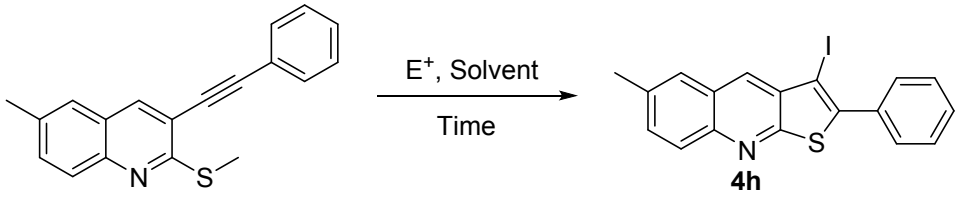
Yield: 76%; Sticky; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.56-7.58 (m, 2H), 7.53 (s, 1H), 7.34-7.40 (m, 5H), 2.76 (s, 3H), 2.61 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 157.31, 146.40, 139.93, 136.36, 132.70, 131.13, 129.59, 128.57, 128.47, 125.86, 125.53, 125.44, 125.10, 121.57, 117.21, 84.06, 77.67, 17.70, 6.21.

2-(Methylselanyl)-3-(phenylbuta-1,3-diyn-1-yl)quinoline (3q)



Yield: 70%; Melting point: 124-126 ^{0}C; IR (neat): 2963, 2211, 1725, 1614, 1578, 1552, 1395, 1354, 1261, 1131, 1063, 912, 859, 799, 753, 688, 636, 526 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.95 (d, *J* = 8.5 Hz, 1H), 7.65-7.70 (m, 2H), 7.58 (dd, *J* = 8.1, 1.3 Hz, 2H), 7.46 (t, *J* = 7.0 Hz, 1H), 7.35-7.41 (m, 3H), 2.61 (t, *J* = 5.8 Hz, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 158.63, 147.70, 139.60, 132.72, 130.82, 129.64, 128.59, 128.23, 127.65, 126.11, 125.27, 121.51, 117.59, 84.20, 81.13, 76.80, 73.67, 6.21; HRMS (ESI): m/z = 348.0291 calcd. For $C_{20}H_{14}NSe$, found 348.0271 $[M+H]^{+}$.

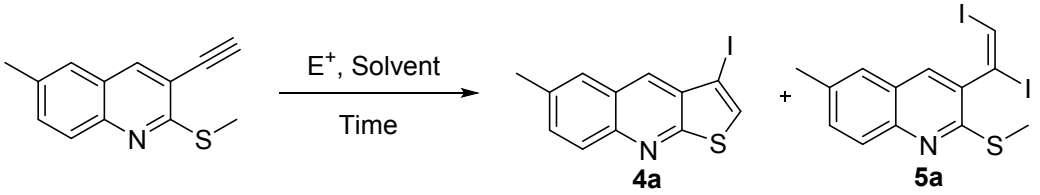
Table S1. Standardization Table for 3-iodo-6-methyl-2-phenylthieno[2,3-b]quinoline 4h:



4h

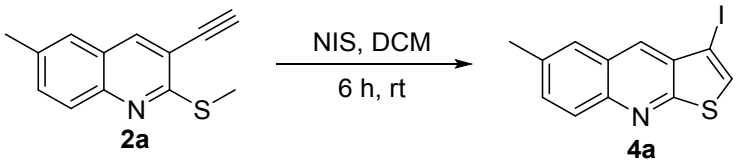
Sr. No.	Solvent	E^+	Time	4h Yield (%)
1	DCM	I_2 (1 eq.)	12	79
2	DCM	I_2 (1.5 eq.)	8	87
3	DCM	I_2 (2 eq.)	6	90
4	DCM	NIS (2 eq.)	6	83
5	THF	I_2 (2 eq.)	14	61
6	$CHCl_3$	I_2 (2 eq.)	8	79
7	DMSO	I_2 (2 eq.)	6	58
8	MeOH	I_2 (2 eq.)	12	72
9	ACN	I_2 (2 eq.)	8	76
10	Toluene	I_2 (2 eq.)	12	79

Table S2. Standardization Table for synthesis of 3-iodo-6-methylthieno[2,3-b]quinoline 4a:



Sr. No.	Solvent	E^+ (2 eq.)	Base	Time	Temp.	Yield (%)	
						4a	5a
1	DCM	I_2	-	6	rt	25	23
2	DCM	I_2	K_2CO_3	6	rt	32	traces
3	DCM	NIS	-	6	rt	69	traces
4	Toluene	NIS		6	90	54	-
5	ACN	NIS	-	12	90	56	-
6	DCM	ICl	-	6	12	-	21
7	Toluene	NIS	K_2CO_3	6	90	39	-

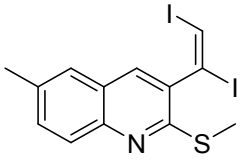
General procedure for synthesis of compounds 4a-4g, 5a, 5b, 5d and 7a-7f:



2a **4a**

To a stirred solution of 3-ethynyl-6-methyl-2-(methylthio)quinoline **2a** (30 mg, 0.140 mmol, 1 equiv.), NIS (63 mg, 0.281 mmol, 2 equiv.) in dry DCM (5 mL) was stirred for 6 h, After completion of reaction (monitored by TLC), reaction mixture was quenched by saturated sodium thiosulfate and extracted with DCM (15 mL). Solvent was evaporated under reduced pressure to afford a crude residue. The crude was purified by silica gel chromatography using hexane/ethyl acetate (98:2) as eluent to afford **4a** 32 mg as white solid, Yield: 69%; Melting point: 176-178 ^{0}C; IR (neat): 3086, 1595, 1548, 1488, 1330, 1136, 1055, 912, 790, 773, 699, 628, 562, 504 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.33 (s, 1H), 8.06 (d, *J* = 9.0 Hz, 1H), 7.78 (s, 1H), 7.75 (s, 1H), 7.62 (d, *J* = 9.0 Hz, 1H), 2.58 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 159.59, 146.03, 135.95, 132.74, 131.77, 131.16, 127.84, 127.07, 126.08, 75.15, 21.76; HRMS (ESI): m/z = 325.9500 calcd. For $C_{12}H_9NSI$, found 325.9511 $[M+H]^+$.

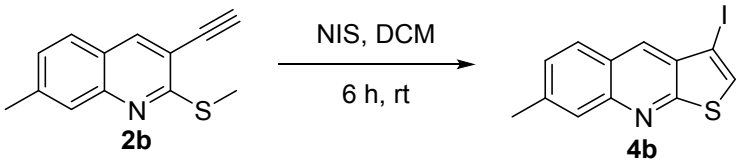
(E)-3-(1,2-diiodovinyl)-6-methyl-2-(methylthio)quinoline (5a)



5a

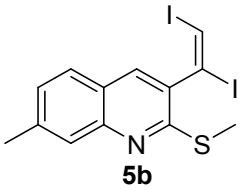
Yield: 23%; Sticky; IR (KBr): 2923, 2367, 2341, 1554, 1490, 1334, 1155, 1052, 824 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.87 (d, *J* = 9.4 Hz, 1H), 7.69 (s, 1H), 7.52 (d, *J* = 6.7 Hz, 2H), 7.49 (s, 1H), 2.70 (s, 3H), 2.51 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 155.29, 146.40, 136.07, 135.60, 134.13, 132.71, 127.75, 126.95, 125.32, 91.41, 87.37, 21.54, 13.40; HRMS (ESI): m/z = 467.8780 calcd. For $C_{13}H_{12}NSI_2$, found 467.8780 $[M+H]^+$.

3-Iodo-7-methylthieno[2,3-b]quinoline (4b)



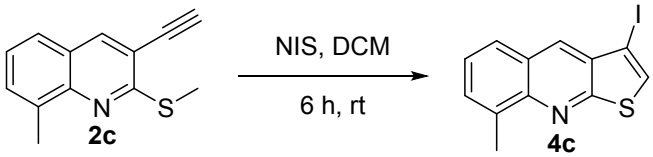
Yield: 70%; Melting point: 130-133 ^{0}C; IR (neat): 2931, 1931, 1732, 1619, 1604, 1573, 1385, 1360, 1259, 1091, 1049, 1040, 809, 797, 779, 766, 697, 574 cm^{-1}; 1H-NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 7.92 (d, *J* = 8.5 Hz, 2H), 7.73 (s, 1H), 7.43 (d, *J* = 9.9 Hz, 1H), 2.62 (s, 3H); 13 C-NMR (100 MHz, $CDCl_3$) δ 160.52, 147.56, 140.74, 132.23, 132.12, 130.63, 128.62, 128.15, 127.00, 124.19, 75.14, 22.24; HRMS (ESI): m/z = 325.9500 calcd. For $C_{12}H_9NSI$, found 325.9496 $[M+H]^+$.

(E)-3-(1,2-diiodovinyl)-7-methyl-2-(methylthio)quinoline (5b)



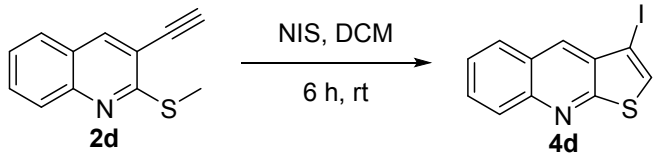
Yield: 21%; Melting point: 99-102 ^{0}C; IR (neat): 3076, 2915, 1904, 1730, 1693, 1605, 1625, 1395, 1327, 1311, 1258, 1088, 1057, 1010, 816, 795, 780, 688 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.77 (s, 1H), 7.72 (s, 1H), 7.64 (d, *J* = 8.1 Hz, 1H), 7.49 (s, 1H), 7.30 (s, 1H), 2.70 (s, 3H), 2.54 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 156.31, 147.97, 141.10, 135.31, 134.40, 127.94, 127.67, 127.28, 123.30, 91.51, 87.41, 22.05, 13.40; HRMS (ESI): m/z = 467.8780 calcd. For $C_{13}H_{12}NSI_2$, found 467.8759 $[M+H]^+$.

3-Iodo-8-methylthieno[2,3-b]quinoline (4c)



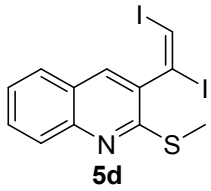
Yield: 72%; Melting point: 179-182 ^{0}C; IR (neat): 2917, 2551, 1971, 1944, 1684, 1614, 1592, 1562, 1544, 1330, 1165, 1093, 889, 762, 558, 488 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.40 (s, 1H), 7.88 (d, *J* = 8.5 Hz, 1H), 7.77 (s, 1H), 7.63 (d, *J* = 6.7 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 1H), 2.88 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 159.56, 146.60, 136.25, 132.64, 132.36, 131.31, 130.00, 126.53, 125.97, 125.83, 74.96, 18.53; HRMS (ESI): m/z = 325.9500 calcd. For $C_{12}H_9INS$, found 325.9529 $[M+H]^+$.

3-Iodothieno[2,3-b]quinoline (4d)



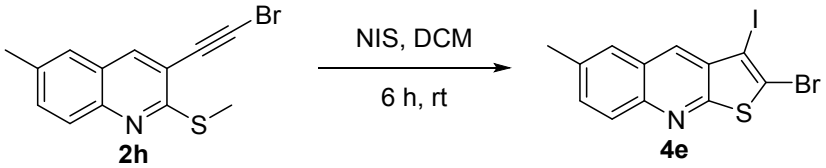
Yield: 61%; Melting point: 152-154 ^{0}C; IR (neat): 3084, 1798, 1586, 1542, 1388, 1325, 1051, 948, 901, 769, 742, 701, 594, 503 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 8.18 (d, *J* = 8.1 Hz, 1H), 8.04 (d, *J* = 7.6 Hz, 1H), 7.79 (m, 2H), 7.61 (m, 1H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.52, 147.23, 132.74, 132.55, 131.41, 130.18, 128.57, 128.25, 126.09, 125.99, 75.10; HRMS (ESI): m/z = 311.9344 calcd. For $C_{11}H_7NSI$, found 311.9362 $[M+H]^+$.

(E)-3-(1,2-diiodovinyl)-2-(methylthio)quinoline (5d)



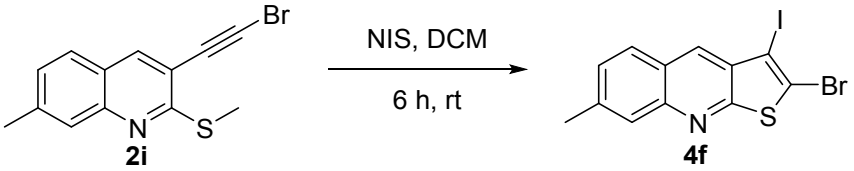
Yield: 20%; Melting point: 135-138 ^{0}C; IR (neat): 2922, 1732, 1603, 1549, 1309, 1380, 1139, 1043, 952, 963, 813, 778, 747, 596, 477 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.1 Hz, 1H), 7.74-7.77 (m, 2H), 7.69 (m, 1H), 7.51 (s, 1H), 7.46 (t, *J* = 6.7 Hz, 1H), 2.71 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 156.50, 147.77, 136.16, 134.62, 130.53, 128.06, 128.02, 125.76, 125.34, 91.12, 87.51, 13.43; HRMS (ESI): m/z = 453.8624 calcd. For $C_{12}H_{10}NSI_2$, found 453.8594 $[M+H]^+$.

2-Bromo-3-iodo-6-methylthieno[2,3-b]quinoline (4e)



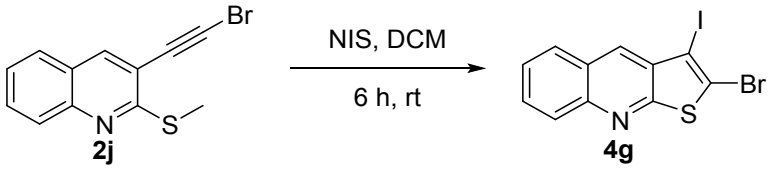
Yield: 81%; Melting point: 134-136 ^{0}C; IR (neat): 2920, 1584, 1551, 1389, 1323, 1136, 1066, 951, 905, 813, 565, 519, 749 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.21 (s, 1H), 8.01 (d, *J* = 8.5 Hz, 1H), 7.76 (s, 1H), 7.62 (d, *J* = 8.5 Hz, 1H), 2.58 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.00, 146.01, 136.38, 133.89, 132.85, 131.97, 127.84, 127.04, 126.62, 122.04, 83.97, 21.76; HRMS (ESI): m/z = 403.8606 calcd. For $C_{12}H_8NSBrI$, found 403.8595 $[M+H]^+$.

2-Bromo-3-iodo-7-methylthieno[2,3-b]quinoline (4f)



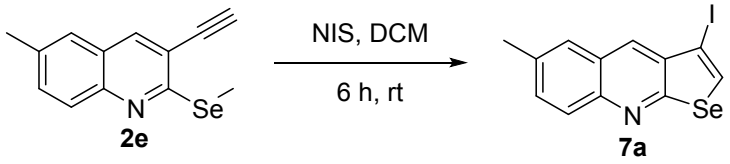
Yield: 85%; Melting point: 201-203 ^{0}C; IR (neat): 1996, 2011, 1705, 1627, 1588, 1549, 1478, 1331, 1308, 1145, 1082, 895, 870, 797, 614, 586, 537, 466 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.24 (s, 1H), 7.88 (d, *J* = 8.5 Hz, 2H), 7.42 (d, *J* = 8.5 Hz, 1H), 2.60 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.91, 147.53, 140.96, 133.28, 132.40, 128.94, 128.08, 127.03, 124.69, 121.43, 83.94, 22.26; HRMS (ESI): m/z = 403.8606 calcd. For $C_{12}H_8NSBrI$, found 403.8590 $[M+H]^+$.

2-Bromo-3-iodothieno[2,3-b]quinoline (4g)



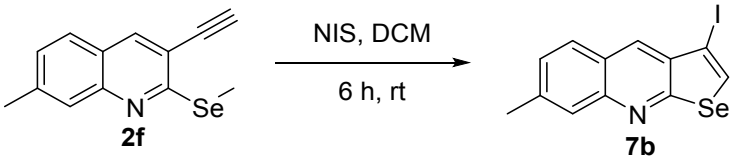
Yield: 84%; Melting point: 178-180 ^{0}C; IR (neat): 2357, 1919, 1801, 1614, 1587, 1547, 1479, 1391, 1321, 1228, 1133, 945, 927, 900, 834, 779, 742, 719, 546, 510 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.31 (s, 1H), 8.07 (dd, *J* = 44.2, 7.9 Hz, 2H), 7.79 (s, 1H), 7.59 (s, 1H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.94, 147.22, 133.91, 132.68, 130.32, 128.49, 128.24, 126.51, 126.45, 122.36, 83.93; HRMS (ESI): m/z = 389.8449 calcd. For $C_{11}H_6NSBrI$, found 389.8420 $[M+H]^+$.

3-Iodo-6-methylselenopheno[2,3-b]quinoline (7a)



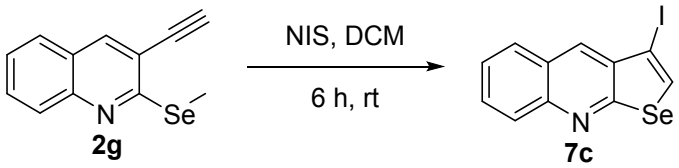
Yield: 64%; Melting point: 181-183 ^{0}C; IR (neat): 3083, 2162, 1778, 1731, 1586, 1527, 1549, 1329, 1263, 1035, 911, 815, 766, 757, 716, 621, 517, 479 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.28 (s, 1H), 8.03 (d, *J* = 9.0 Hz, 1H), 7.77 (s, 1H), 7.62 (d, *J* = 9.0 Hz, 1H), 2.58 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.42, 145.71, 136.09, 135.05, 133.87, 132.78, 132.32, 127.66, 127.21, 126.12, 76.79, 21.76; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 582.01; HRMS (ESI): m/z = 373.8945 calcd. For $C_{12}H_9NSeI$, found 373.8925 $[M+H]^+$.

3-Iodo-7-methylselenopheno[2,3-b]quinoline (7b)



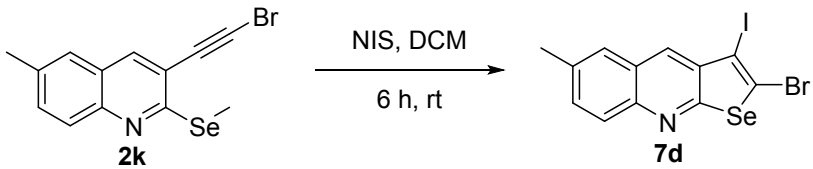
Yield: 54%; Sticky; IR (KBr): 2362, 2347, 1616, 1585, 1555, 1486, 1317, 1132, 753, 669 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.42 (s, 1H), 8.27 (s, 1H), 7.92-7.94 (m, 2H), 7.45 (d, *J* = 8.5 Hz, 1H), 2.62 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 141.04, 134.54, 134.39, 131.86, 128.75, 128.24, 127.23, 126.73, 126.70, 124.22, 77.65, 22.24; ^{77}Se-NMR (75 MHz, $CDCl_3$) δ 631.83; HRMS (ESI): m/z = 373.8945 calcd. For $C_{12}H_9NSeI$, found 373.8959 $[M+H]^+$.

3-Iodoselenopheno[2,3-b]quinoline (7c)



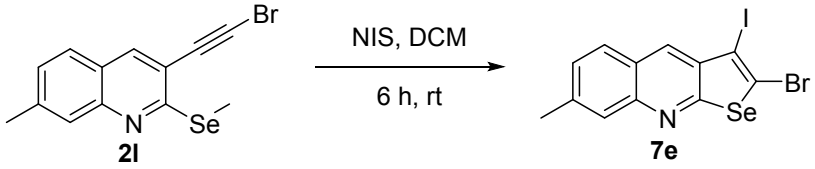
Yield: 60%; Sticky; IR (KBr): 2927, 2854, 2378, 2158, 1676, 1616, 1486, 1137, 1048, 956, 914, 860, 752, 668, 583 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.32 (s, 1H), 8.16 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 7.79-7.83 (m, 1H), 7.61 (t, *J* = 7.6 Hz, 1H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 162.49, 146.92, 135.13, 134.57, 132.58, 130.29, 128.65, 128.05, 126.23, 126.06, 76.77; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 584.41; HRMS (ESI): m/z = 359.8788 calcd. For $C_{11}H_7NSeI$, found 359.8797 $[M+H]^+$.

2-Bromo-3-iodo-6-methylselenopheno[2,3-b]quinoline (7d)



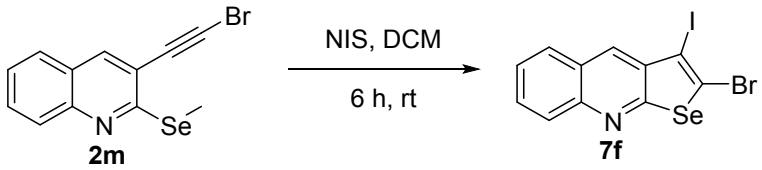
Yield: 75%; Melting point: 187-188 ^{0}C; IR (neat): 2917, 1682, 1584, 1567, 1548, 1488, 1392, 1329, 1259, 1099, 1061, 1028, 909, 813, 782, 763, 631, 480 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.20 (s, 1H), 7.92 (d, *J* = 8.5 Hz, 1H), 7.69 (s, 1H), 7.55 (d, *J* = 9.0 Hz, 1H), 2.51 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 163.58, 146.02, 136.50, 136.30, 134.38, 132.89, 127.64, 127.20, 126.78, 120.54, 87.58, 21.75; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 661.99; HRMS (ESI): m/z = 451.8050 calcd. For $C_{12}H_8NSeBrI$, found 451.8061 $[M+H]^+$.

2-Bromo-3-iodo-7-methylselenopheno[2,3-b]quinoline (7e)



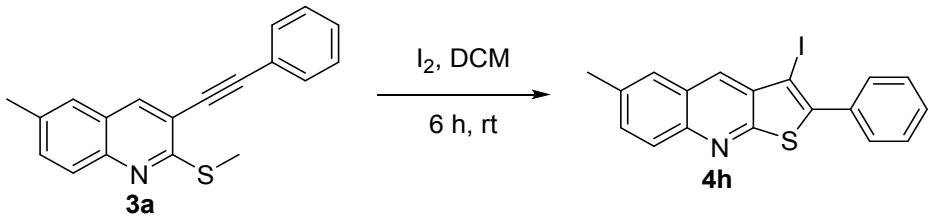
Yield: 61%; Melting point: 203-206 ^{0}C; IR (neat): 1800, 1614, 1587, 1547, 1322, 1134, 945, 900, 774, 741, 597, 546, 473 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$ and Acetone-d_6) δ 8.27 (d, *J* = 4.6 Hz, 1H), 7.78-7.85 (m, 2H), 7.38 (d, *J* = 8.2 Hz, 1H), 2.53 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$ and Acetone-d_6) δ 147.19, 141.34, 135.80, 135.02, 129.07, 128.16, 128.12, 126.33, 124.82, 119.90, 87.43, 22.07; ^{77}Se-NMR (400 MHz, $CDCl_3$ and Acetone-d_6) δ 664.55; HRMS (ESI): m/z = 451.8050 calcd. For $C_{12}H_8NSeBrI$, found 451.8031 $[M+H]^+$.

2-Bromo-3-iodoselenopheno[2,3-b]quinoline (7f)



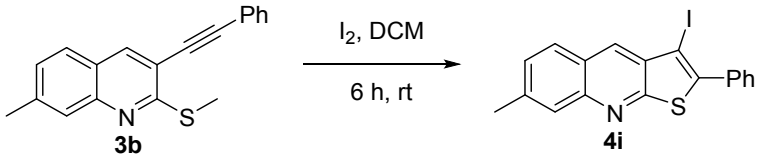
Yield: 71%; Melting point: 178-182 ^{0}C; IR (neat): 2923, 2028, 1733, 1613, 1581, 1551, 1326, 1316, 1140, 1129, 1070, 900, 892, 823, 752, 742, 496, 474 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 8.02 (d, *J* = 8.5 Hz, 1H), 7.81 (t, *J* = 7.0 Hz, 1H), 7.61 (t, *J* = 8.1 Hz, 1H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 164.66, 147.25, 136.39, 135.04, 130.43, 128.59, 128.04, 126.72, 126.58, 120.89, 87.48; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 664.24; HRMS (ESI): m/z = 437.7894 calcd. For $C_{11}H_6NSeBrI$, found 437.7906 $[M+H]^+$.

General procedure for the synthesis of 4h-4q and 7g-7m:



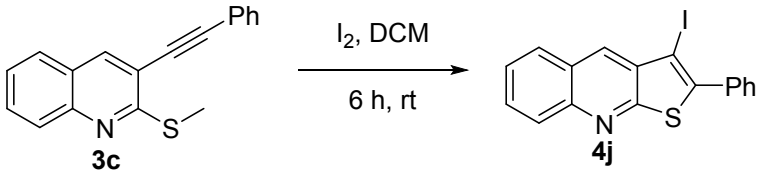
To a stirred solution of 6-methyl-2-(methylthio)-3-(phenylethynyl)quinoline **3a** (10 mg, 0.034 mmol, 1 equiv.) and iodine (18 mg, 0.069 mmol, 2 equiv.) in dry DCM (5 mL) was stirred for 6 h, After completion of reaction (monitored by TLC), reaction mixture was quenched by saturated sodium thiosulfate and extracted with DCM (15 mL). Solvent was evaporated under reduced pressure to afford a crude residue. The crude was purified by silica gel chromatography using hexane/ethyl acetate (97:3) as eluent to afford **4h** as white crystal, Yield: 90%; Melting point: 183-186 ^{0}C; IR (neat): 2916, 1674, 1629, 1588, 1575, 1550, 1488, 1440, 1181, 1093, 1074, 902, 839, 814, 754, 693, 569, 558 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.39 (s, 1H), 8.07 (d, *J* = 9.0 Hz, 1H), 7.81 (s, 1H), 7.76 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.62 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.48-7.54 (m, 3H), 2.59 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.44, 146.29, 143.53, 135.83, 135.23, 134.41, 133.18, 132.55, 132.48, 130.41, 130.00, 129.52, 128.75, 127.81, 127.09, 126.67, 75.93, 21.76; HRMS (ESI): m/z = 401.9813 calcd. For $C_{18}H_{13}NSI$, found 401.9842 $[M+H]^+$.

3-Iodo-7-methyl-2-phenylthieno[2,3-b]quinoline (4i)



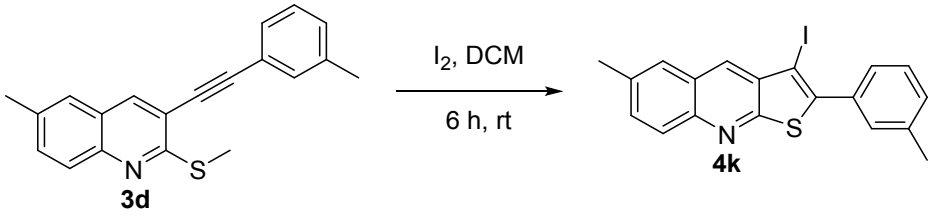
Yield: 79%; Melting point: 143-146 ^{0}C; IR (neat): 2914, 2373, 1631, 1530, 1474, 1440, 1304, 1144, 1073, 897, 868, 795, 758, 737, 691, 616, 598, 465 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 7.93-7.95 (m, 2H), 7.76 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.48-7.54 (m, 3H), 7.43 (d, *J* = 9.9 Hz, 1H), 2.63 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.35, 147.82, 142.93, 140.58, 134.63, 134.42, 132.92, 130.00, 129.48, 128.74, 128.50, 128.13, 127.00, 124.76, 75.91, 22.24; HRMS (ESI): m/z = 401.9813 calcd. For $C_{18}H_{13}NSI$, found 401.9835 $[M+H]^+$.

3-Iodo-2-phenylthieno[2,3-b]quinoline (4j)



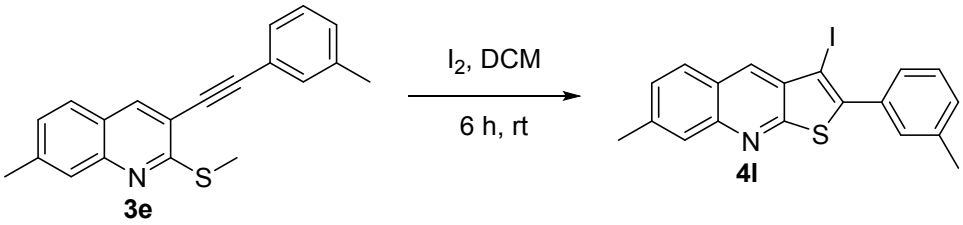
Yield: 86%; Melting point: 163-166 ^{0}C; IR (neat): 2922, 1613, 1583, 1548, 1476, 1327, 1143, 1075, 891, 853, 836, 762, 748, 738, 694, 599, 470 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 8.18 (d, *J* = 8.5 Hz, 1H), 8.05 (d, *J* = 8.1 Hz, 1H), 7.76-7.81 (m, 3H), 7.59 (t, *J* = 7.0 Hz, 1H), 7.49-7.55 (m, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.36, 147.49, 143.69, 135.25, 134.33, 133.21, 130.01, 129.59, 128.77, 128.54, 128.19, 126.56, 125.99, 75.86; HRMS (ESI): m/z = 387.9657 calcd. For $C_{17}H_{11}NSI$, found 387.9656 $[M+H]^+$.

3-Iodo-6-methyl-2-(m-tolyl)thieno[2,3-b]quinoline (4k)



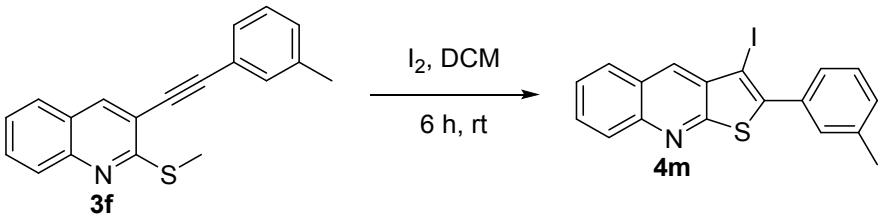
Yield: 83%; Melting point: 156-160 ^{0}C; IR (neat): 2913, 1809, 1771, 1582, 1548, 1487, 1335, 1138, 1083, 1075, 904, 815, 793, 728, 698, 565, 478 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.38 (s, 1H), 8.06 (d, *J* = 9.0 Hz, 1H), 7.80 (s, 1H), 7.59 (q, *J* = 9.0 Hz, 3H), 7.40 (t, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 7.6 Hz, 1H), 2.59 (s, 3H), 2.47 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.45, 146.25, 143.67, 138.55, 135.78, 135.24, 134.30, 132.49, 132.39, 130.56, 130.30, 128.62, 127.80, 127.10, 126.66, 75.75, 21.76, 21.54; HRMS (ESI): m/z = 415.9970 calcd. For $C_{19}H_{15}NSI$, found 415.9976 $[M+H]^+$.

3-Iodo-7-methyl-2-(m-tolyl)thieno[2,3-b]quinoline (4l)



Yield: 80%; Melting point: 104-107 ^{0}C; IR (neat): 2918, 1732, 1624, 1451, 1478, 1333, 1144, 1085, 893, 885, 873, 790, 779, 768, 621, 468 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 7.87 (t, *J* = 4.0 Hz, 2H), 7.50 (d, *J* = 9.0 Hz, 2H), 7.34 (q, *J* = 7.5 Hz, 2H), 7.22 (d, *J* = 7.6 Hz, 1H), 2.55 (s, 3H), 2.40 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.37, 147.78, 143.15, 140.52, 138.55, 134.64, 134.30, 132.84, 130.57, 130.26, 128.61, 128.47, 128.12, 127.10, 126.99, 124.75, 75.72, 22.24, 21.54; HRMS (ESI): m/z = 415.9970 calcd. For $C_{19}H_{15}INS$, found 415.9969 $[M+H]^+$.

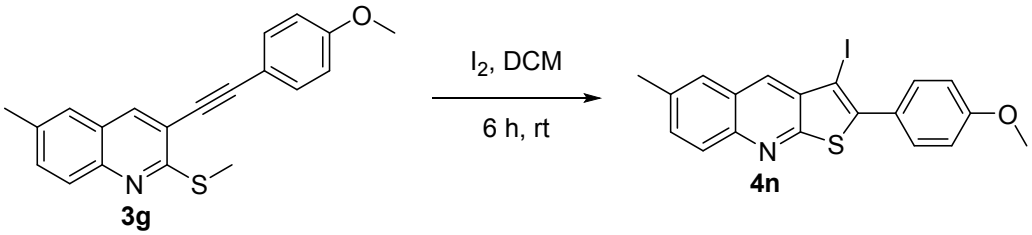
3-Iodo-2-(m-tolyl)thieno[2,3-b]quinoline (4m)



3f 4m

Yield: 86%; Melting point: 131-134 ^{0}C; IR (neat): 3052, 1806, 1615, 1600, 1548, 1329, 1128, 1084, 899, 851, 805, 771, 746, 694, 736, 599, 475 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 8.17 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 9.0 Hz, 1H), 7.75-7.79 (m, 1H), 7.56-7.60 (m, 3H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 7.6 Hz, 1H), 2.47 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.37, 147.45, 143.91, 138.59, 135.26, 134.21, 133.11, 130.56, 130.38, 129.96, 128.65, 128.52, 128.18, 127.11, 126.56, 125.95, 75.67, 21.55; HRMS (ESI): m/z = 401.9813 calcd. For $C_{18}H_{13}NSI$, found 401.9803 $[M+H]^+$.

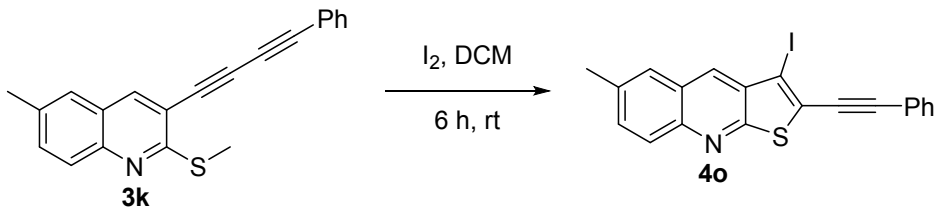
3-Iodo-2-(4-methoxyphenyl)-6-methylthieno[2,3-b]quinoline (4n)



3g 4n

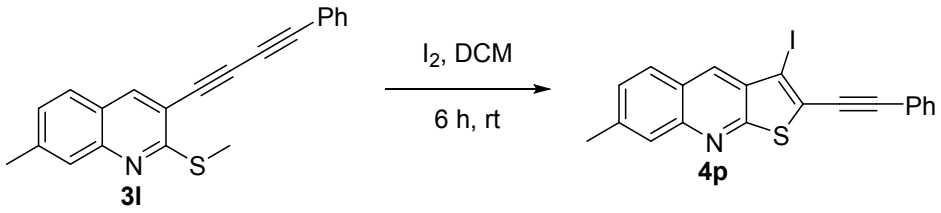
Yield: 77%; Melting point: 178-180 ^{0}C; IR (neat): 2988, 1775, 1731, 1605, 1490, 1459, 1435, 1295, 1252, 1178, 1112, 1087, 1027, 825, 813, 792, 764, 559, 525 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 8.06 (d, *J* = 9.0 Hz, 1H), 7.80 (s, 1H), 7.72 (d, *J* = 8.5 Hz, 2H), 7.61 (d, *J* = 9.0 Hz, 1H), 7.04 (d, *J* = 8.5 Hz, 2H), 3.90 (s, 3H), 2.59 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.60, 146.12, 143.40, 135.77, 135.41, 132.40, 132.13, 131.36, 127.75, 127.06, 126.69, 126.64, 114.17, 75.09, 55.52, 21.76; HRMS (ESI): m/z = 431.9919 calcd. For $C_{19}H_{15}NOS$, found 431.9924 $[M+H]^+$.

3-Iodo-6-methyl-2-(phenylethynyl)thieno[2,3-b]quinoline (4o)



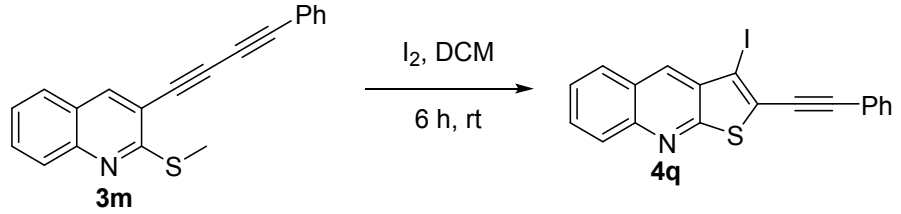
Yield: 81%; Melting point: 208-211 ^{0}C; IR (neat): 2206, 1728, 1678, 1588, 1548, 1488, 1440, 1331, 1135, 1070, 907, 864, 816, 792, 757, 690, 560, 554 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 8.04 (d, *J* = 8.5 Hz, 1H), 7.77 (s, 1H), 7.64-7.67 (m, 2H), 7.61 (d, *J* = 9.0 Hz, 1H), 7.40-7.42 (m, 3H), 2.58 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 159.94, 146.81, 136.13, 133.59, 132.92, 132.23, 131.95, 129.59, 128.64, 127.83, 127.17, 126.54, 126.20, 122.05, 101.17, 84.71, 84.36, 21.75; HRMS (ESI): m/z = 425.9813 calcd. For $C_{20}H_{13}NSI$, found 425.9788 $[M+H]^+$.

3-Iodo-7-methyl-2-(phenylethynyl)thieno[2,3-b]quinoline (4p)



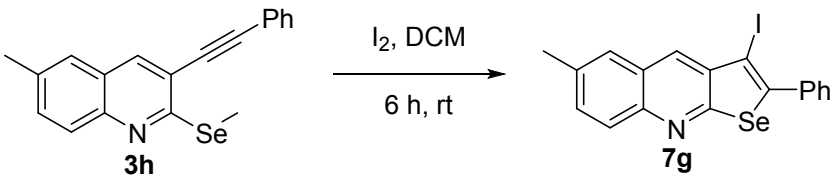
Yield: 84%; Melting point: 212-215 ^{0}C; IR (neat): 2920, 2163, 1911, 1688, 1625, 1590, 1545, 1439, 1331, 1148, 1071, 895, 888, 878, 787, 760, 693, 593, 545 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 7.90 (t, *J* = 4.0 Hz, 2H), 7.64-7.66 (m, 2H), 7.40-7.42 (m, 4H), 2.61 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.86, 148.30, 141.05, 132.96, 132.67, 131.93, 129.56, 128.74, 128.63, 128.22, 127.01, 125.66, 124.63, 122.08, 101.01, 84.75, 84.36, 22.29; HRMS (ESI): m/z = 425.9813 calcd. For $C_{20}H_{13}NSI$, found 425.9827 $[M+H]^+$.

3-Iodo-2-(phenylethynyl)thieno[2,3-b]quinoline (4q)



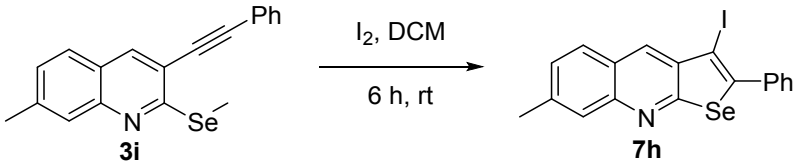
Yield: 91%; Melting point: 222-224 ^{0}C; IR (neat): 2964, 2201, 1813, 1614, 1586, 1546, 1329, 1146, 1128, 1070, 900, 778, 753, 723, 687, 540, 472 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 8.02 (d, *J* = 8.5 Hz, 1H), 7.78 (t, *J* = 7.2 Hz, 1H), 7.64-7.67 (m, 2H), 7.59 (t, *J* = 7.2 Hz, 1H), 7.40-7.43 (m, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 160.88, 147.99, 133.62, 132.97, 131.97, 130.37, 129.65, 128.65, 128.22, 126.45, 126.24, 121.99, 101.41, 84.63, 84.29, 76.78; HRMS (ESI): m/z = 411.9657 calcd. For $C_{19}H_{11}NSI$, found 411.9632 $[M+H]^+$

3-Iodo-6-methyl-2-phenylselenopheno[2,3-b]quinoline (7g)



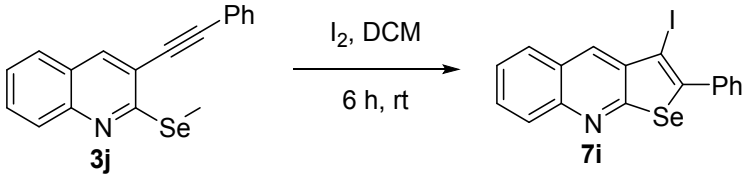
Yield: 79%; Melting point: 179-182 ^{0}C; IR (neat): 2920, 2345, 1805, 1718,1674, 1571, 1549, 1488, 1438, 1333, 1301, 902, 814, 767, 704, 745, 692,556, 513 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.44 (s, 1H), 8.04 (d, *J* = 8.5 Hz, 1H), 7.80 (s, 1H), 7.68 (dd, *J* = 8.1, 1.3 Hz, 2H), 7.62 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.46-7.52 (m, 3H), 2.59 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 162.82, 146.16, 145.59, 137.86, 136.81, 136.04, 134.74, 132.69, 130.07, 129.36, 128.76, 127.68, 127.32, 126.86, 76.85, 21.84; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 628.19; HRMS (ESI): m/z = 449.9258 calcd. For $C_{18}H_{13}NSeI$, found 449.9253 $[M+H]^+$.

3-Iodo-7-methyl-2-phenylselenopheno[2,3-b]quinoline (7h)



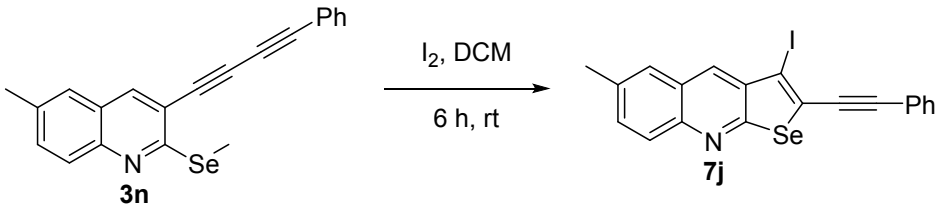
Yield: 86%; Melting point: 129-132 ^{0}C; IR (neat): 2915, 1748, 1622, 1575, 1474, 1440, 1331, 1223, 1057, 898, 798, 761, 692, 593, 468 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.47 (s, 1H), 7.91 (d, *J* = 7.6 Hz, 2H), 7.66-7.68 (m, 2H), 7.45-7.51 (m, 3H), 7.42 (d, *J* = 8.5 Hz, 1H), 2.62 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 163.79, 147.58, 144.96, 140.72, 137.18, 136.72, 135.03, 130.00, 129.25, 128.69, 128.56, 128.21, 126.85, 124.84, 79.03, 22.26; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 629.89; HRMS (ESI): m/z = 449.9258 calcd. For $C_{18}H_{13}NSeI$, found 449.9255 $[M+H]^+$.

3-Iodo-2-phenylselenopheno[2,3-b]quinoline (7i)



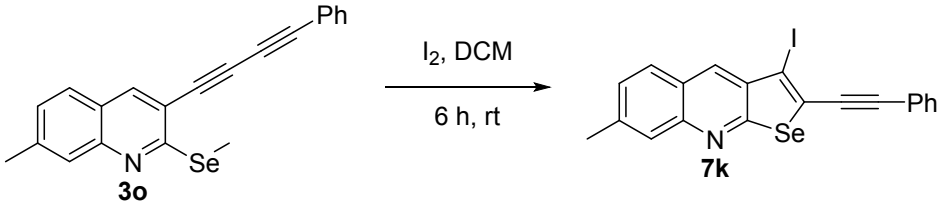
Yield: 85%; Melting point: 139-142 ^{0}C; IR (neat): 2922, 1847, 1819, 1731, 1614, 1577, 1551, 1479, 1441, 1328, 1261, 1133, 1076, 1056, 1027, 760, 742, 690, 606, 465 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 7.77-7.81 (m, 1H), 7.68 (dd, *J* = 7.9, 1.6 Hz, 2H), 7.60 (t, *J* = 7.0 Hz, 1H), 7.47-7.52 (m, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 163.81, 147.28, 145.76, 137.85, 136.64, 135.32, 130.14, 130.00, 129.35, 128.72, 128.62, 127.98, 126.70, 126.11, 78.96; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 630.59; HRMS (ESI): m/z = 435.9101 calcd. For $C_{17}H_{11}NSeI$, found 435.9128 $[M+H]^+$.

3-Iodo-6-methyl-2-(phenylethynyl)selenopheno[2,3-b]quinoline (7j)



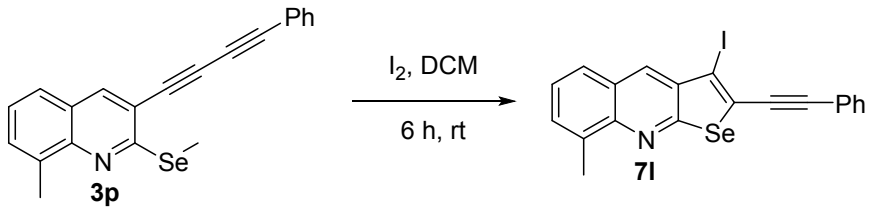
Yield: 79%; Melting point: 200-203 ^{0}C; IR (neat): 2920, 1913, 1722, 1579, 1549, 1479, 1439, 1331, 1136, 902, 856, 814, 753, 697,686, 517, 479 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 1H), 8.00 (d, *J* = 8.5 Hz, 1H), 7.75 (s, 1H), 7.59-7.64 (m, 3H), 7.41 (t, *J* = 2.7 Hz, 3H), 2.57 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 162.17, 146.57, 136.24, 136.17, 134.43, 132.93, 131.85, 129.53, 128.64, 127.62, 127.32, 126.64, 125.74, 122.28, 102.77, 87.42, 86.55, 21.75; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 648.77; HRMS (ESI): m/z = 473.9258 calcd. For $C_{20}H_{13}NSeI$, found 473.9250 $[M+H]^+$.

3-Iodo-7-methyl-2-(phenylethynyl)selenopheno[2,3-b]quinoline (7k)



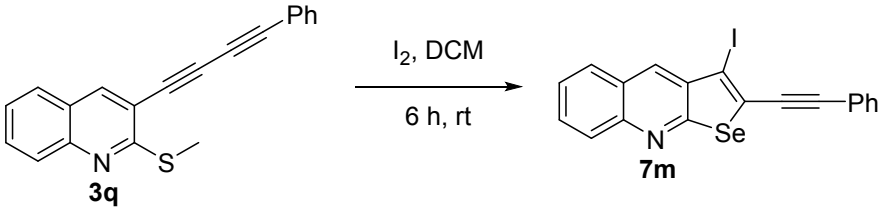
Yield: 80%; Melting point: 183-186 ^{0}C; IR (neat): 3006, 2364, 2348, 2341, 1714, 1427, 1364, 1223, 1093, 895, 798, 687, 529 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.34 (s, 1H), 7.88 (d, *J* = 8.2 Hz, 2H), 7.62-7.65 (m, 2H), 7.41 (q, *J* = 2.9 Hz, 4H), 2.60 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 163.22, 148.05, 141.17, 135.56, 134.82, 131.84, 129.49, 128.79, 128.63, 128.32, 126.88, 125.25, 124.72, 122.32, 102.60, 87.40, 86.56, 22.28; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 650.19; HRMS (ESI): m/z = 473.9258 calcd. For $C_{20}H_{13}NSeI$, found 473.9262 $[M+H]^+$.

3-Iodo-8-methyl-2-(phenylethynyl)selenopheno[2,3-b]quinoline (7l)



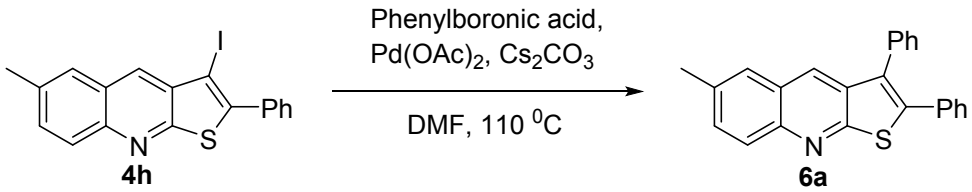
Yield: 87%; Melting point: 231-234 ^{0}C; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.37 (s, 1H), 7.85 (d, *J* = 8.1 Hz, 1H), 7.61-7.66 (m, 3H), 7.48 (d, *J* = 8.1 Hz, 1H), 7.41 (t, *J* = 2.7 Hz, 3H), 2.86 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 162.13, 147.12, 136.15, 135.89, 135.27, 131.85, 130.37, 129.50, 128.63, 126.68, 126.58, 126.08, 122.34, 102.68, 87.31, 86.65, 18.43; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 651.94.

3-Iodo-2-(phenylethynyl)selenopheno[2,3-b]quinoline (7m)



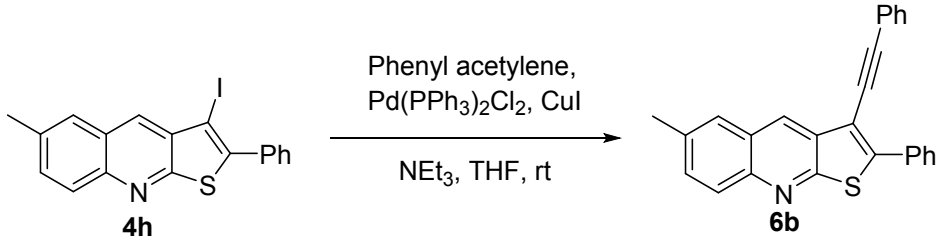
Yield: 85%; Melting point: 194-197 ^{0}C; IR (neat): 2961, 2191, 1729, 1546, 1478, 1439, 1332, 1258, 1069, 1013, 852, 792, 773, 748, 694, 685, 589 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.43 (s, 1H), 8.13 (d, *J* = 8.5 Hz, 1H), 8.03 (d, *J* = 7.6 Hz, 1H), 7.78 (d, *J* = 6.7 Hz, 1H), 7.63-7.66 (m, 2H), 7.60 (s, 1H), 7.42 (q, *J* = 2.4 Hz, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 147.79, 136.27, 135.12, 131.86, 130.45, 129.59, 128.75, 128.66, 128.65, 128.03, 126.59, 126.37, 126.04, 122.22, 103.02, 87.24, 86.48; ^{77}Se-NMR (400 MHz, $CDCl_3$) δ 651.01; HRMS (ESI): m/z = 459.9101 calcd. For $C_{19}H_{11}NSeI$, found 459.9104 $[M+H]^+$.

General procedure for the synthesis of 6-methyl-2,3-diphenylthieno[2,3-b]quinoline (6a)



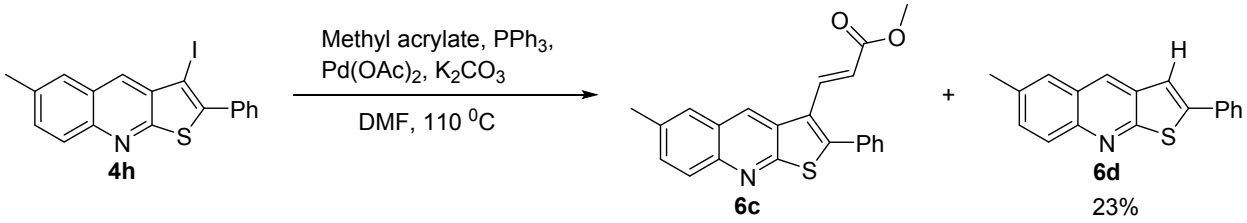
To a solution of 3-iodo-6-methyl-2-phenylthieno[2,3-b]quinoline **4h** (20 mg, 0.050 mmol) the phenyl boronic acid (9.1 mg, 0.075 mmol) in 4 ml DMF, Pd $(OAc)_2$ (1.1 mg, 1 mol %), Cs_2CO_3 (48.7 mg, 0.150 mmol) were added. The resulting mixture was then heated at 60 ^{0}C for 12 h. The solvent was removed under reduced pressure, the residue was extracted with ethyl acetate: brine; The crude was purified by silica gel chromatography using hexane/ethyl acetate (95:5) as eluents to afford **6a** 13 mg, Yield: 74%; Melting point: 186-188 ^{0}C; IR (neat): 2917, 1978, 1626, 1599, 1584, 1556, 1491, 1442, 1298, 1357, 1090, 908, 820, 755, 698, 559, 478 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 8.05 (d, *J* = 9.0 Hz, 1H), 7.62 (s, 1H), 7.56-7.58 (m, 1H), 7.42-7.48 (m, 3H), 7.39 (td, *J* = 3.9, 1.9 Hz, 4H), 7.28 (t, *J* = 3.1 Hz, 3H), 2.53 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 161.42, 145.65, 140.23, 135.23, 134.84, 134.10, 133.84, 131.98, 130.38, 130.25, 129.85, 129.13, 129.05, 128.57, 128.43, 127.94, 127.92, 127.08, 126.09, 21.71; HRMS (ESI): m/z = 352.1160 calcd. For $C_{24}H_{18}NS$, found 352.1159 $[M+H]^+$.

General procedure for synthesis of 6-methyl-2-phenyl-3-(phenylethynyl)thieno[2,3-b]quinoline (6b)



To a solution of the corresponding 3-iodo-6-methyl-2-phenylthieno[2,3-b]quinoline **4h** (0.062 mmol) and the phenyl acetylene (0.080 mmol, 1.3 equiv) in 5ml THF; Et_3N (1 mL), $PdCl_2(PPh_3)_2$ (4.4 mg, 1 mol %) and copper(I) iodide (1.19 mg, 1 mol %) were added. The resulting mixture was then stirred under nitrogen atmosphere for 14 h. The solvent was removed under reduced pressure, the residue was extracted with ethyl acetate and purified by silica gel column chromatography using hexane: ethyl acetate (97:3) as eluent to afford **6b** 18 mg, Yield: 77%; Melting point: 129-131 ^{0}C; IR (neat): 2919, 1791, 1732, 1624, 1587, 1478, 1451, 1333, 1261, 1445, 897, 790, 778, 768, 694, 621, 468 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 8.14 (d, *J* = 7.2 Hz, 2H), 8.05 (d, *J* = 8.5 Hz, 1H), 7.78 (s, 1H), 7.62-7.64 (m, 2H), 7.59 (d, *J* = 9.0 Hz, 1H), 7.52 (t, *J* = 7.4 Hz, 2H), 7.41-7.47 (m, 4H), 2.58 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 159.82, 147.11, 146.11, 135.69, 133.71, 133.66, 132.25, 131.75, 129.59, 129.18, 128.88, 128.76, 128.64, 128.04, 127.11, 126.78, 126.24, 123.10, 110.78, 95.36, 83.41, 21.75; HRMS (ESI): m/z = 376.1160 calcd. For $C_{26}H_{18}NS$, found 376.1154 $[M+H]^+$.

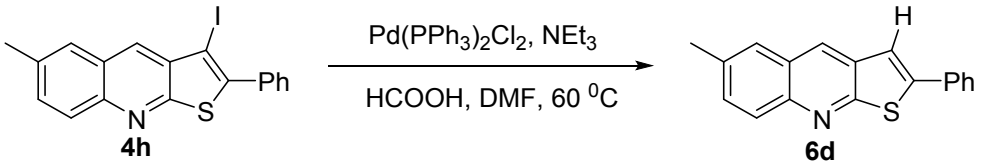
General procedure for the synthesis of methyl (E)-3-(6-methyl-2-phenylthieno[2,3-b]quinolin-3-yl)acrylate (6c)



To a solution of the corresponding 3-iodo-6-methyl-2-phenylthieno[2,3-b]quinoline **4h** (20 mg, 0.037 mmol) and the methyl acrylate (6.5 mg, 0.074 mmol) in 4 ml DMF; Pd $(OAc)_2$ (0.4 mg, 0.5 mol %), PPh_3 (9.8 mg, 0.037 mmol) and K_2CO_3 (10.3 mg, 0.074 mmol) were added. The resulting mixture was then heated under nitrogen atmosphere for 12 h. The solvent was removed under reduced pressure, the residue was extracted with ethyl acetate and purified by silica gel column chromatography using hexane: ethyl acetate (97:3) as eluent to afford **6c** 12 mg, along with 23% **6d**; Yield: 70%; Melting point: 186-190 ^{0}C; IR (neat): 2917, 1716, 1627, 1587, 1491, 1443, 1423, 1305, 1283, 1222, 1174, 1158, 1080, 1095, 1013, 898, 817, 691, 563 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.70 (s, 1H), 8.05 (d, *J* = 8.5 Hz, 1H), 7.90 (d, *J* = 16.2 Hz, 1H), 7.78 (s, 1H), 7.58-7.63 (m, 3H), 7.51 (t, *J* = 7.4 Hz, 3H), 6.66 (d, *J* = 16.6 Hz, 1H), 3.85 (s, 3H), 2.60 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 167.65, 161.09, 148.79, 145.54, 137.42, 135.89, 133.14, 132.52, 130.87,

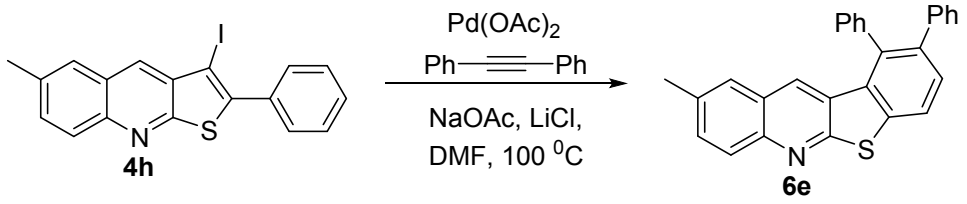
130.28, 129.73, 129.33, 129.07, 127.94, 127.22, 126.06, 124.18, 119.96, 51.95, 21.76; HRMS (ESI): m/z = 360.1058 calcd. For $C_{22}H_{18}NO_2S$, found 360.1057 $[M+H]^+$.

General procedure for the synthesis of 6-methyl-2-phenylthieno[2,3-b]quinoline (6d)



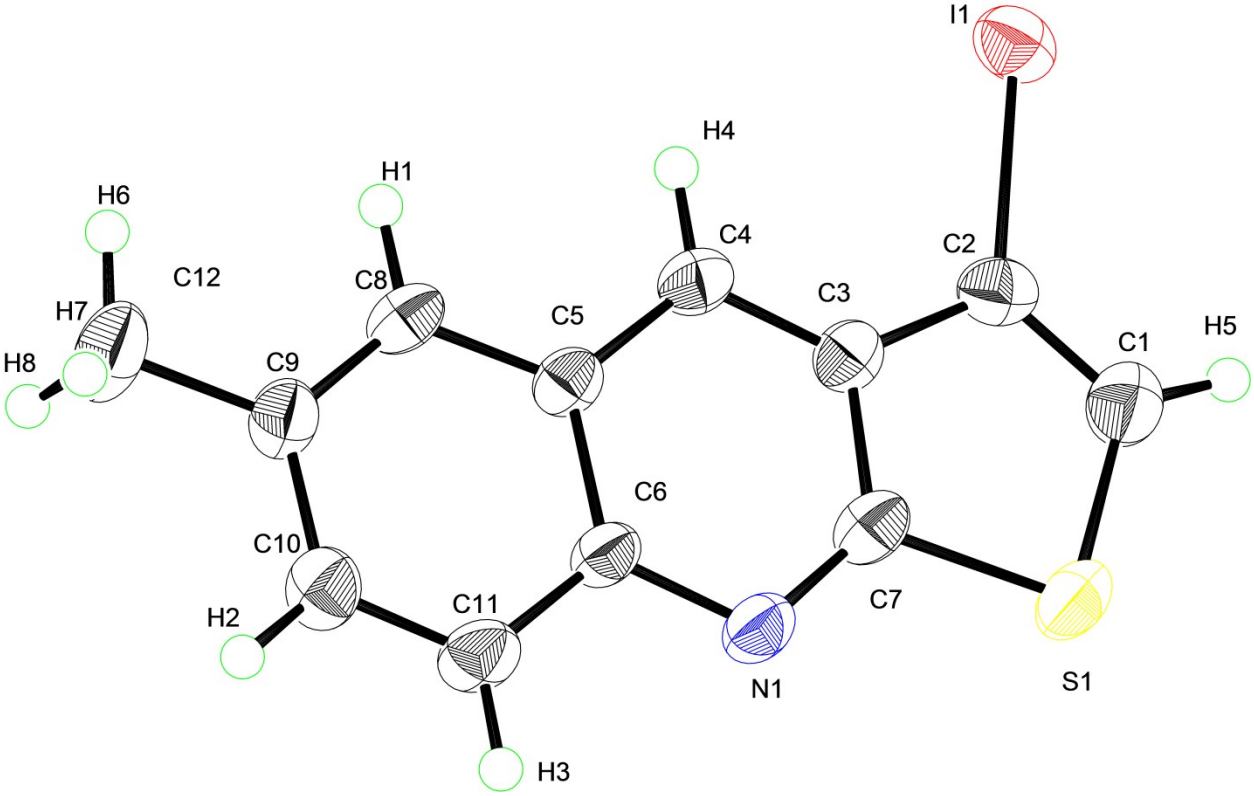
To a solution of the corresponding 3-iodo-6-methyl-2-phenylthieno[2,3-b]quinoline **4h** (30 mg, 0.074 mmol) the formic acid (6.9 mg, 0.149 mmol) in 5 ml DMF, Pd $(PPh_3)_2Cl_2$ (2.6 mg, 0.5 mol %), NEt_3 (22.7 mg, 0.224 mmol) were added. The resulting mixture was then heated at 60^0C for 12 h. The solvent was removed under reduced pressure, the residue was extracted with ethyl acetate: brine and purified by silica gel column chromatography using hexane: ethyl acetate (98:2) as eluent to afford **6d** 16 mg, Yield: 78%; Melting point: 239-243 ^{0}C; IR (neat): 1738, 1646, 1625, 1587, 1552, 1533, 1489, 1444, 1341, 1217, 1068, 913, 903, 817, 750, 680, 700, 691, 560, 473 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.36 (s, 1H), 8.02 (d, *J* = 9.0 Hz, 1H), 7.76-7.78 (m, 2H), 7.68 (s, 1H), 7.54-7.57 (m, 2H), 7.47 (dd, *J* = 8.1, 6.7 Hz, 2H), 7.41 (d, *J* = 7.2 Hz, 1H), 2.56 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 162.35, 145.45, 145.24, 135.35, 133.95, 133.45, 131.79, 129.15, 128.86, 128.05, 126.88, 126.79, 126.21, 116.24, 21.72; HRMS (ESI): m/z = 275.0769 calcd. For $C_{18}H_{13}NS$, found 275.0746 $[M+H]^+$.

General procedure for the synthesis of 9-methyl-1,2-diphenylbenzo[4,5]thieno[2,3-b]quinoline (6e)



To a solution of 3-iodo-6-methyl-2-phenylthieno[2,3-b]quinoline **4h** (20 mg, 0.049 mmol), Pd $(OAc)_2$ (0.6 mg, 5 mol %), NaOAc (8 mg, 0.099 mmol), LiCl (6 mg, 0.149 mmol), in 4 mL DMF; Diphenylacetylene (9 mg, 0.049 mmol) were added. The resulting mixture was heated at 100 °C for 4 days. The mixture was allowed to cool to room temperature, diluted with diethyl ether (15 mL); dried over sodium sulfate, and filtered. The solvent was removed under reduced pressure and the residue was purified by column chromatography using hexane: ethyl acetate (98:2) as eluent to afford **6e** 11 mg (49%) as a yellow solid; Melting point: >300 ^{0}C; IR (neat): 1961, 1801, 1601, 1585, 1548, 1493, 1439, 1327, 1256, 1103, 1070, 1030, 911, 823, 813, 755, 726, 698, 564 cm^{-1}; ^{1}H-NMR (400 MHz, $CDCl_3$) δ 8.25 (d, *J* = 8.1 Hz, 1H), 7.99 (d, *J* = 8.5 Hz, 1H), 7.65 (d, *J* = 8.5 Hz, 1H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.52 (d, *J* = 8.5 Hz, 2H), 7.39 (d, *J* = 5.8 Hz, 3H), 7.26-7.29 (m, 5H), 7.20-7.24 (m, 2H), 7.16 (s, 1H), 6.99 (s, 1H), 2.47 (s, 3H); ^{13} C-NMR (100 MHz, $CDCl_3$) δ 162.09, 145.48, 139.61, 138.41, 137.11, 136.88, 135.89, 135.10, 132.22, 132.16, 131.35, 131.31, 130.37, 130.24, 128.66, 128.26, 128.15, 128.07, 127.72, 127.63, 127.50, 127.48, 127.32, 126.82, 126.81, 125.23, 125.20, 21.54; HRMS (ESI): m/z = 452.1496 calcd. For $C_{32}H_{22}NS$, found 452.1473 $[M+H]^+$.

Figure S1. ORTEP diagram of 3-iodo-6-methylthieno[2,3-b]quinoline (4a).



CCDC 1565817 for **4a** contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Table S3. Crystal data and structure refinement for 3-iodo-6-methylthieno[2,3-b]quinoline (4a)

Empirical formula	$C_{12}H_8INS$
Formula weight	325.15
Temperature(K)	296(2)
Crystal system	Monoclinic
Space group	$P2_1/a$
Unit cell dimensions	
a (Å)	14.189(14)
b (Å)	4.122(4)
c (Å)	19.078 (19)
Volume (Å^3)	1109.3(19)
Z	4
Density calculated (g/m^3)	1.947
F(000)	624
Crystal size (mm^3)	0.20 x 0.20 x 0.20
θ range for data collection (°)	2.89-27.50
Limiting indices	-10<=*h*<=18,-5<=*k*<=5,-24<=*l*<=15
Reflection collected	4593
Independent reflections	2461 (*R*int = 0.0407)
Refinement method	full-matrix least-squares on F^2
Goodness-of-fit on F^2	0.809
Final *R* indices [$I > 2a$ (I)]	*R*1 = 0.0470, *wR*2 = 0.1189
R indices (all data)	*R*1 = 0.0607, *wR*2 = 0.1346
Largest difference peak and hole	1.827 and -1.479 (e Å^{-3})

Computational detail

All stationary point structures of the reactions were optimized by M06-2X DFT method.[1] The 6-31G* electronic basis set was adopted for all atoms except for iodine and bromine. For iodine[2] and bromine, Midi! electronic basis set was adopted. Solvent effect (CH_2Cl_2) was taken into account by SCRF-PCM method,[3] and ultrafine integration grid (specified by Int(Grid=UltraFine) keyword in GAUSSIAN 09 program[4]) was used for all DFT calculations to enhance calculation accuracy. Normal mode analyses were performed to characterize these optimized structures and to obtain thermal correction to Gibbs free energy at T = 298.15 K. We confirm that all structures have the appropriate number of imaginary frequencies; 0 for minimum and 1 for transition state (TS) structures. Then we calculated M06-2X/6-311+G**+Midi! energies at the M06-2X/6-31G*+Midi! optimized geometries to obtain more accurate electronic energies. All calculations were performed with the aid of GAUSSIAN 09 program.[4]

References for computational detail

(1) Zhao, Y.; Truhlar D. G., *Theor. Chem. Acc.* **2006**, *120*, 215-241.
(2) Chen, C.-C.; Wu, M.-Y., Chen, H.-Y.; Wu, M.-J. *J. Org. Chem.* **2017**, *82*, 6071-6081.
(3) Tomasi, J.; Mennucci, B.; Cammi, R. *Chem. Rev.* **2005**, *105*, 2999-3093.
(4) Frisch, M. J.; *et al.* Gaussian 09, Revision B.01; Gaussian, Inc.: Wallingford CT, 2010.

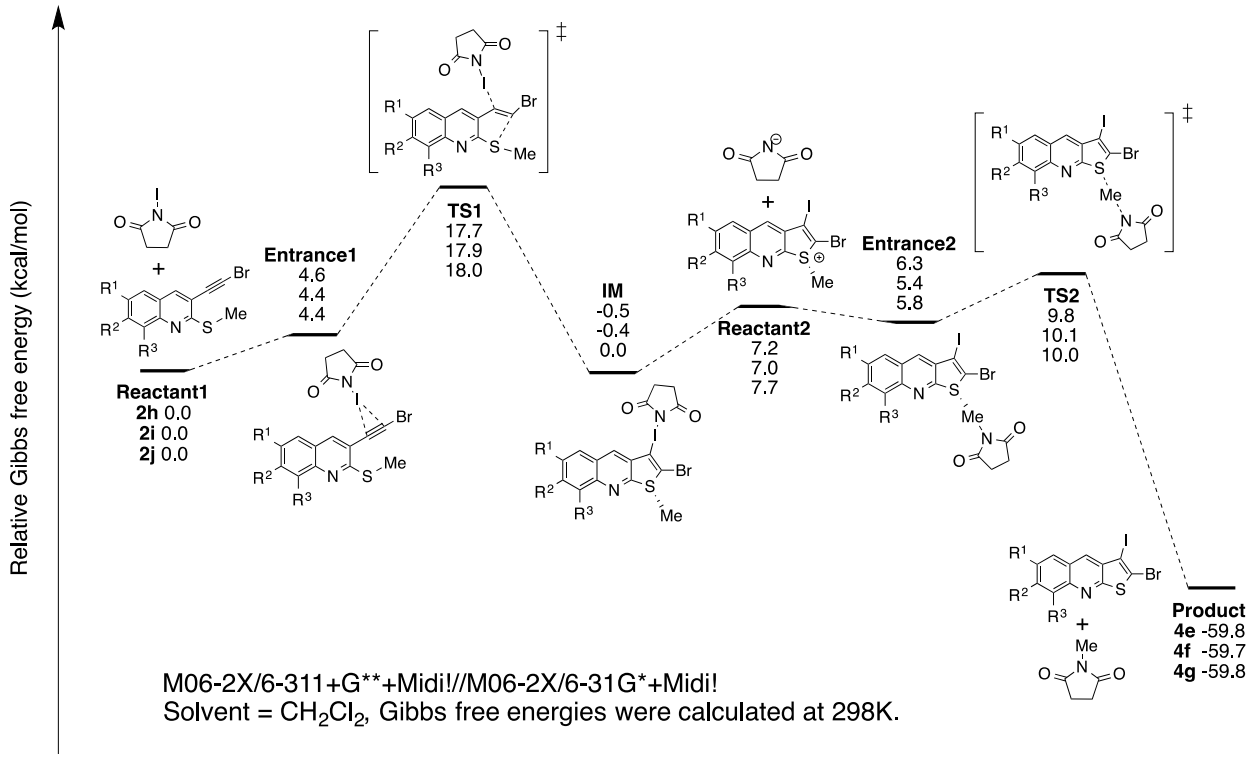


Figure S2. Relative Gibbs free energy profiles of the reactions leading to **4e**-**4g**.

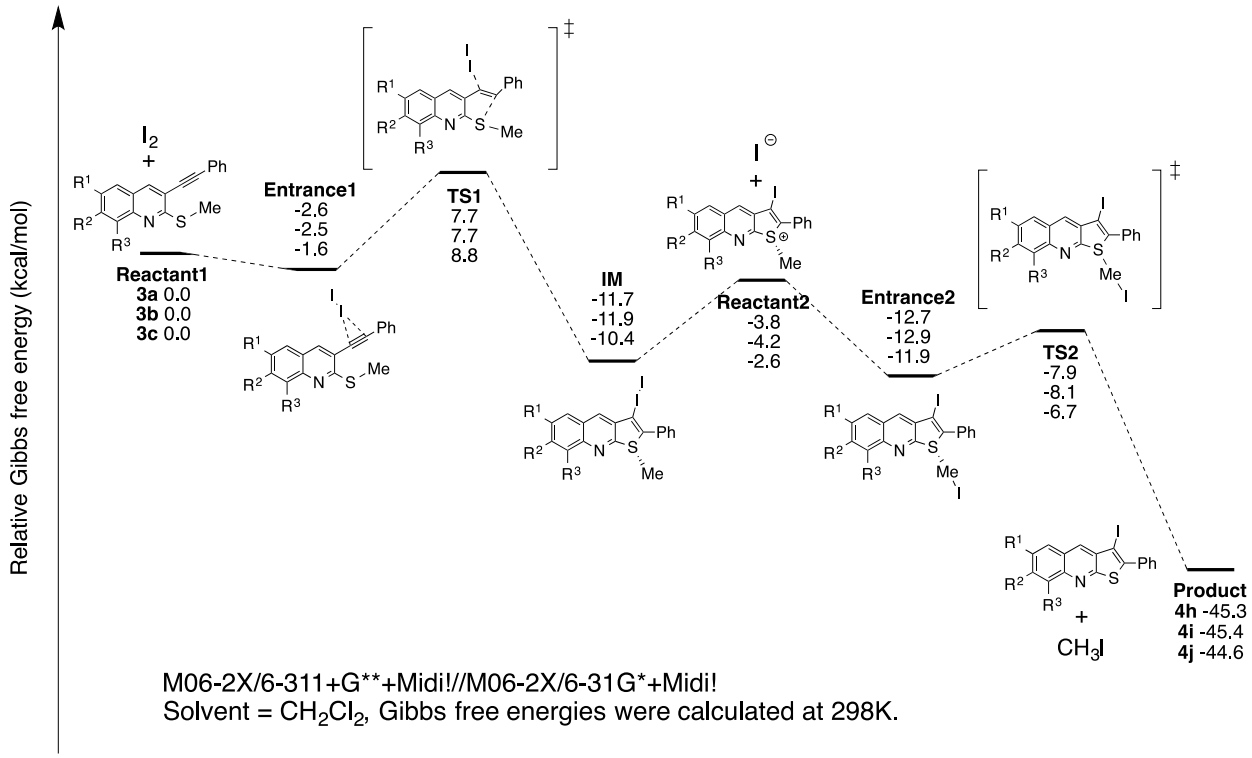


Figure S3. Relative Gibbs free energy profiles of the reactions leading to **4h**-**4j**.

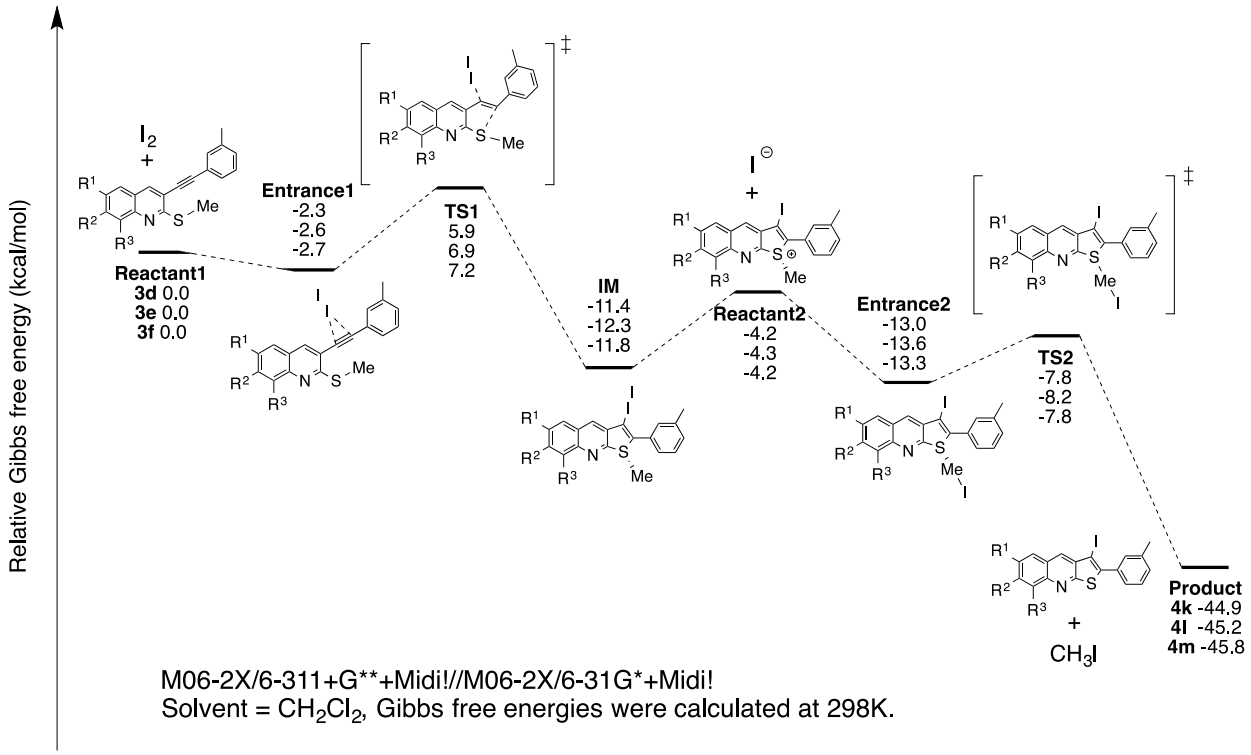


Figure S4. Relative Gibbs free energy profiles of the reactions leading to **4k**-**4m**.

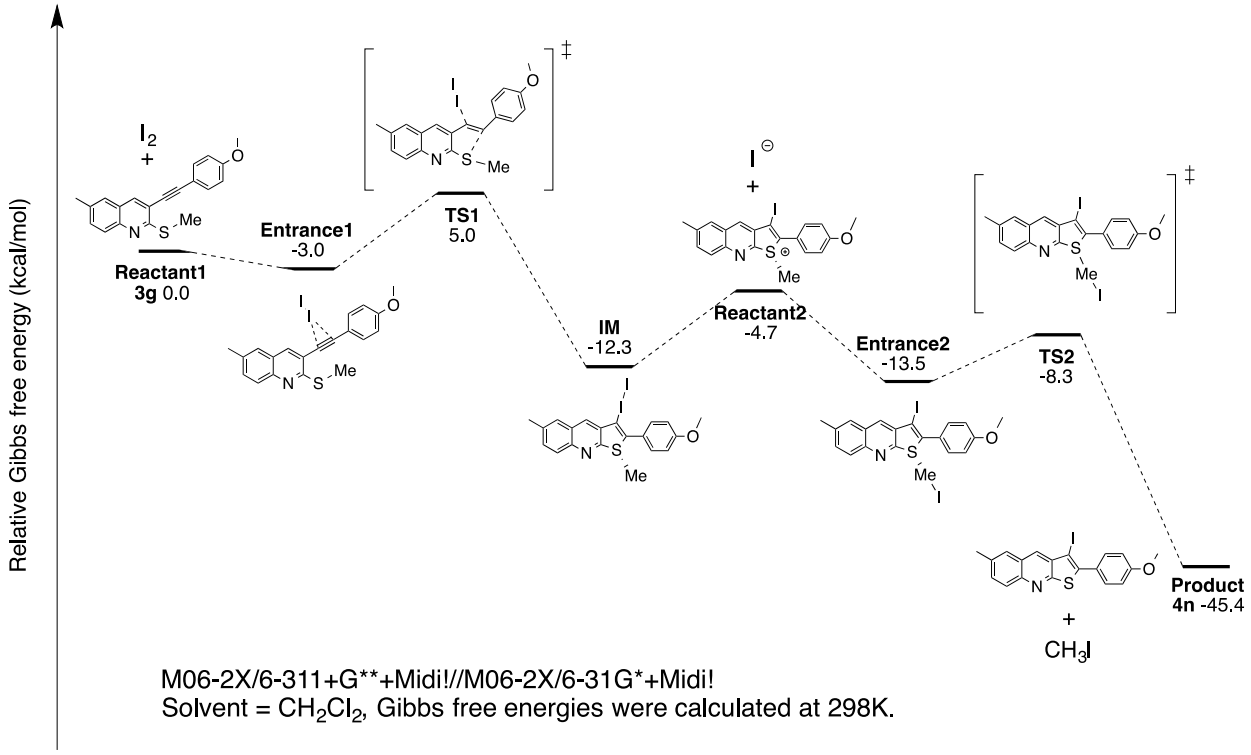


Figure S5. Relative Gibbs free energy profiles of the reactions leading to **4n**.

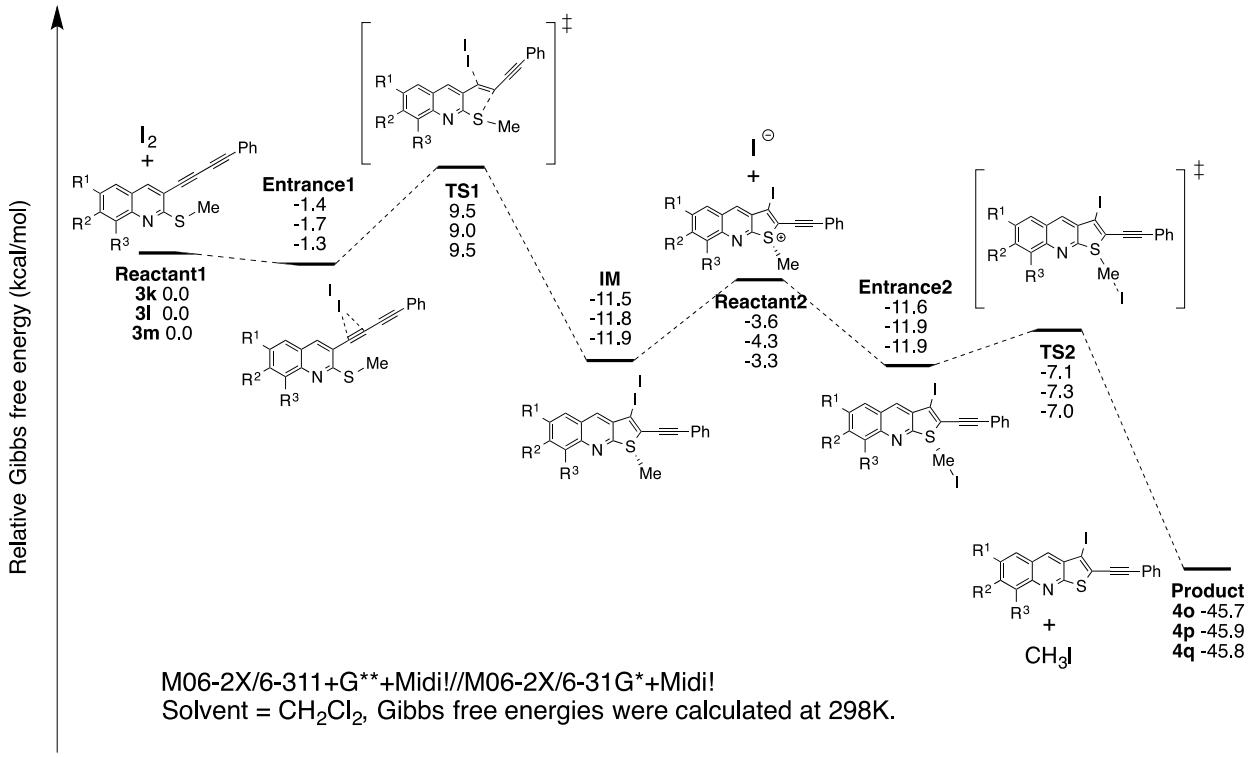
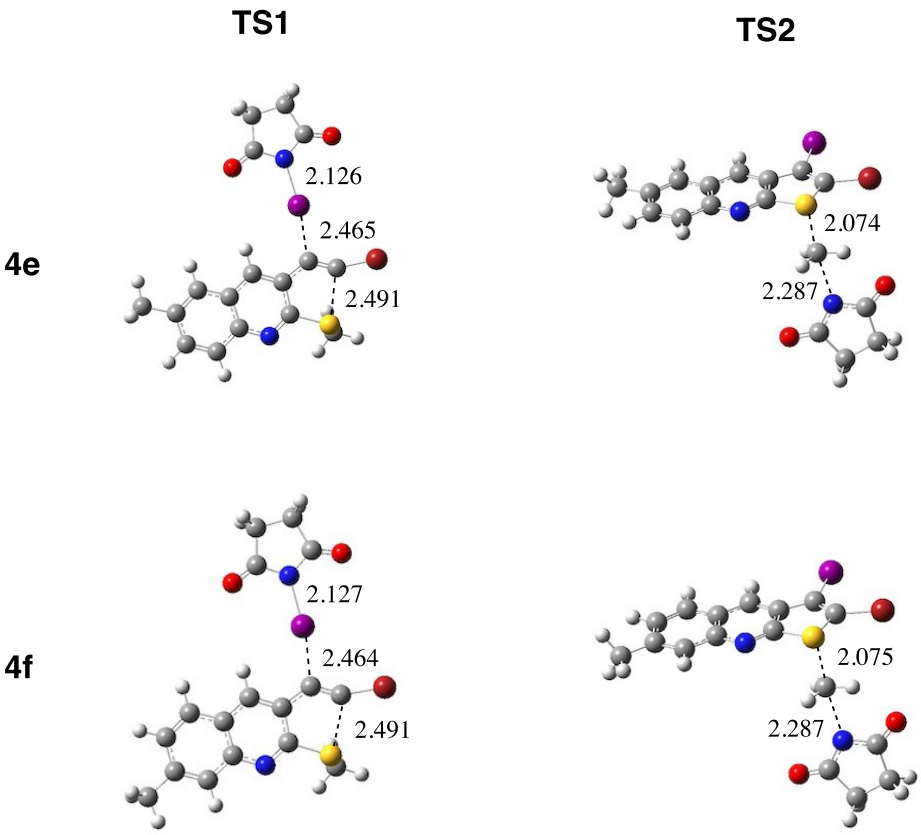
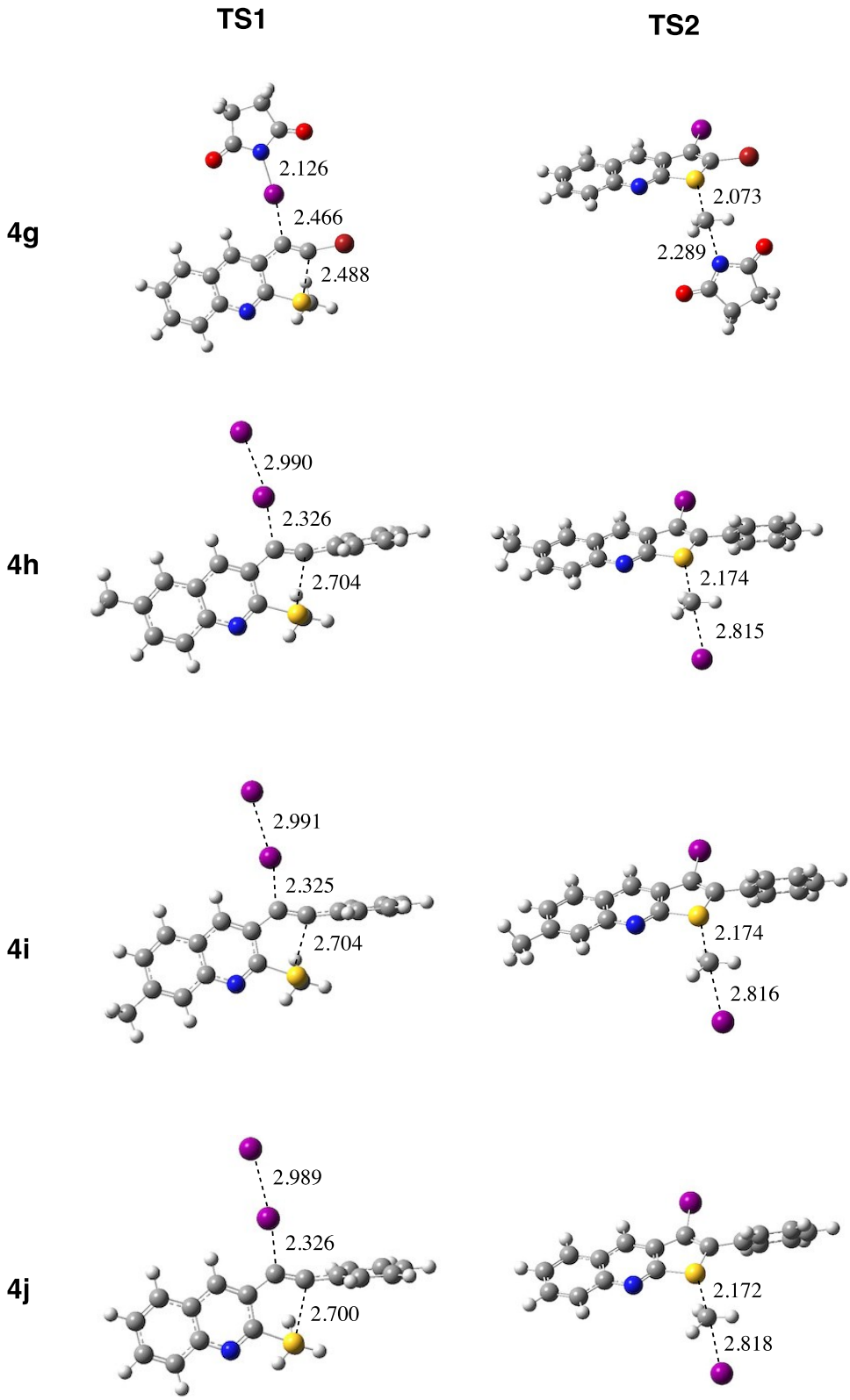
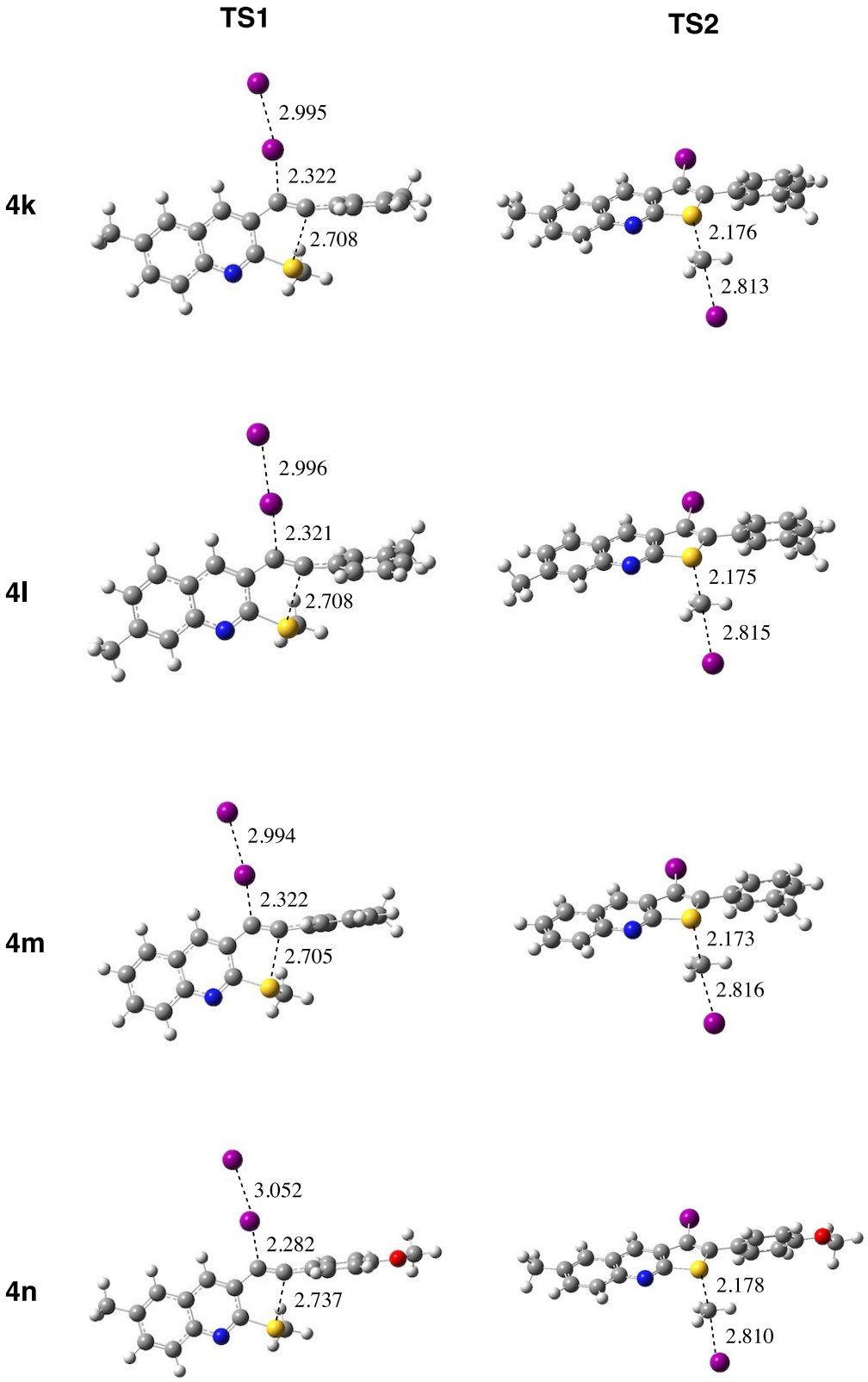


Figure S6. Relative Gibbs free energy profiles of the reactions leading to **4o**-**4q**.




TS1
TS2
4g
2.126
2.466
2.488
2.073
2.289
4h
2.990
2.326
2.704
2.174
2.815
4i
2.991
2.325
2.704
2.174
2.816
4j
2.989
2.326
2.700
2.172
2.818


TS1
TS2
4k
2.995
2.322
2.708
2.176
2.813
4l
2.996
2.321
2.708
2.175
2.815
4m
2.994
2.322
2.705
2.173
2.816
4n
3.052
2.282
2.737
2.178
2.810

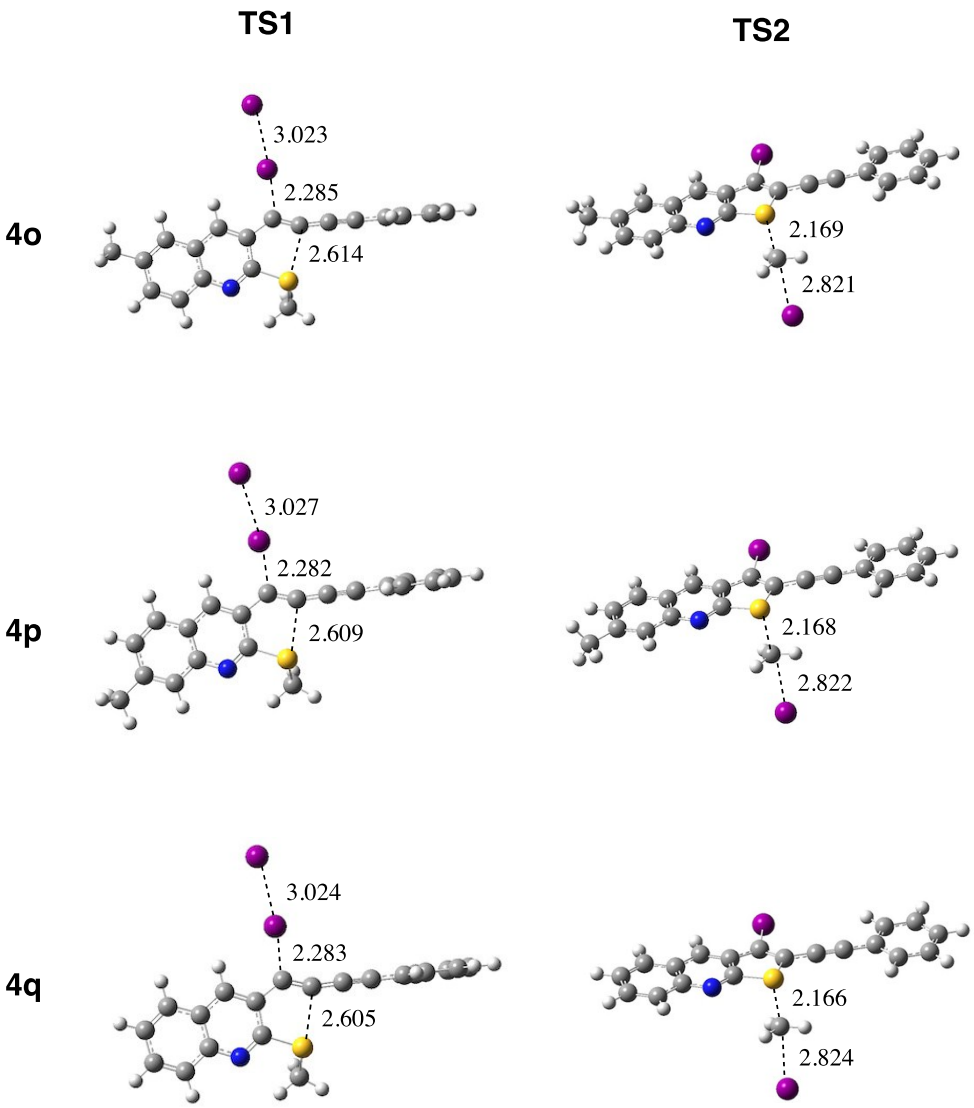


Figure S7. M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi!-optimized geometries (parameters are in [Å]) of **TS1** and **TS2** of the reactions leading to **4e**-**4q**.

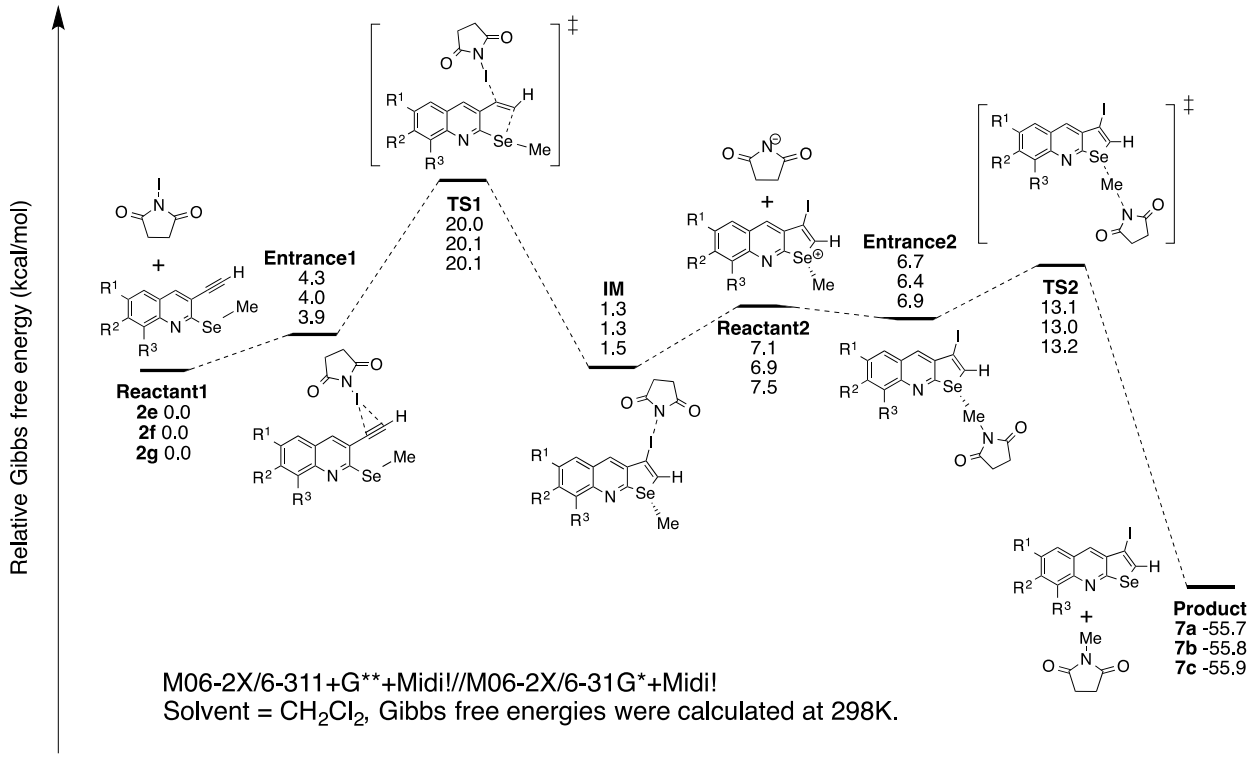


Figure S8. Relative Gibbs free energy profiles of the reactions leading to **7a**-**7c**.

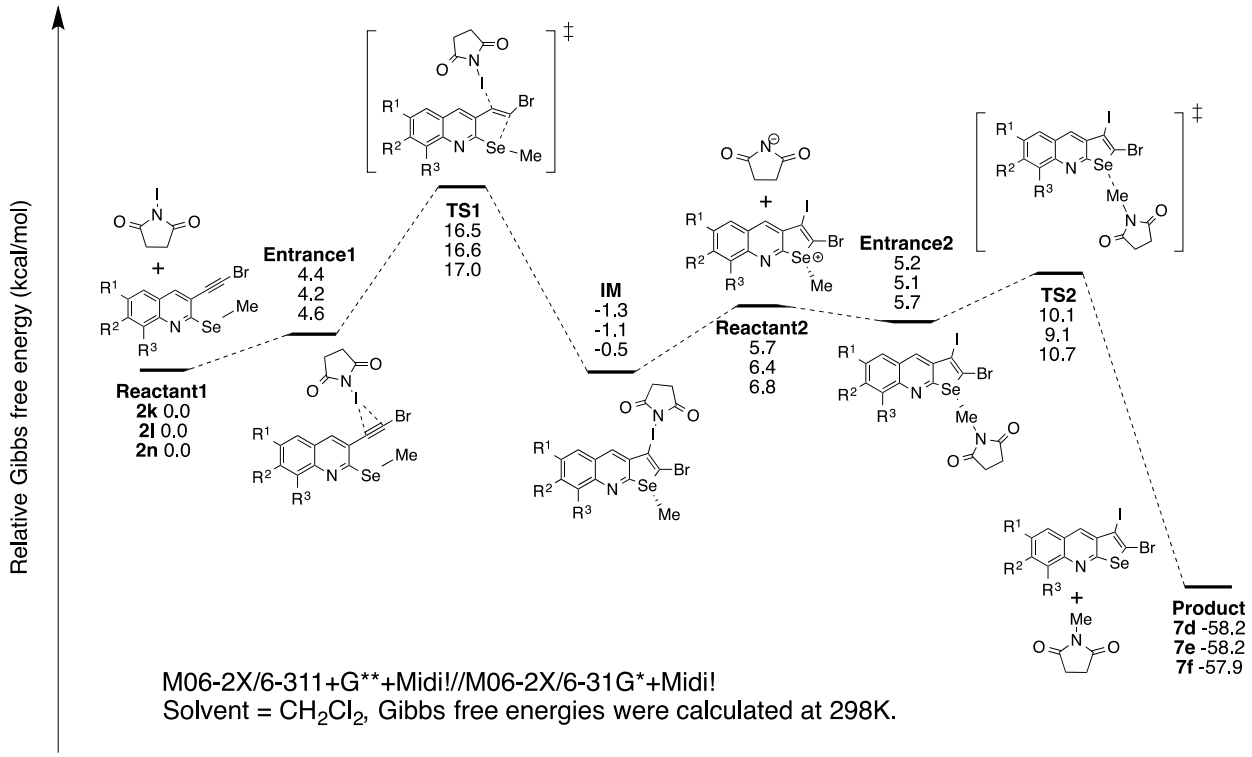


Figure S9. Relative Gibbs free energy profiles of the reactions leading to **7d**-**7f**.

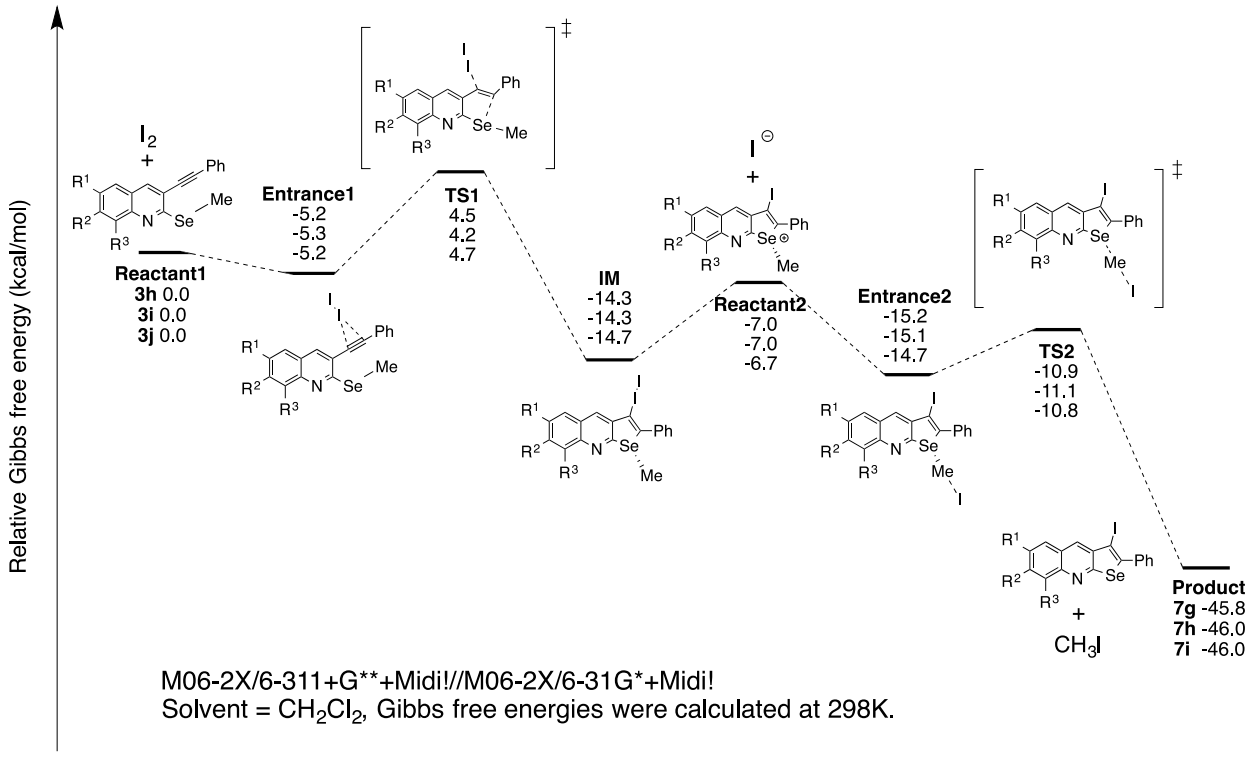


Figure S10. Relative Gibbs free energy profiles of the reactions leading to **7g**-**7i**.

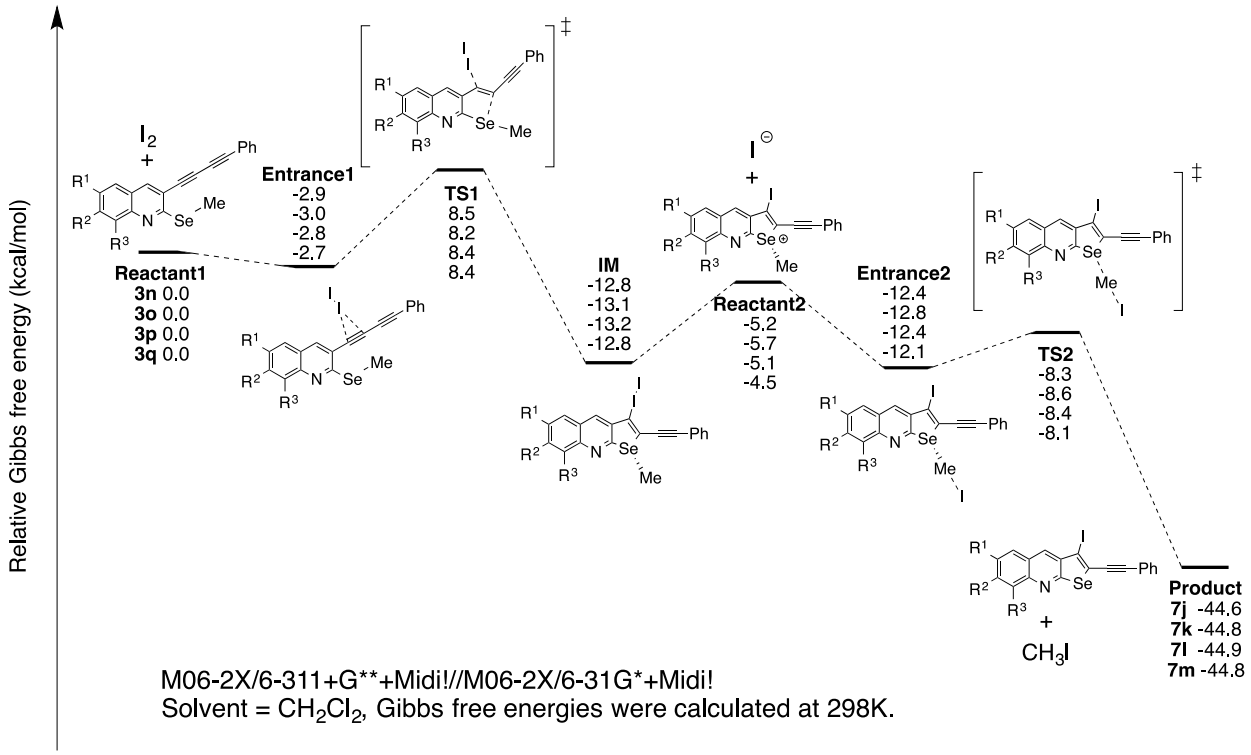
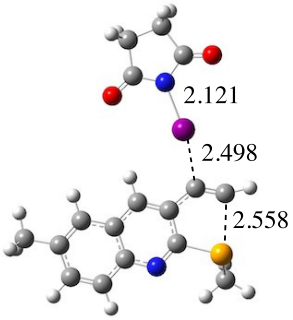
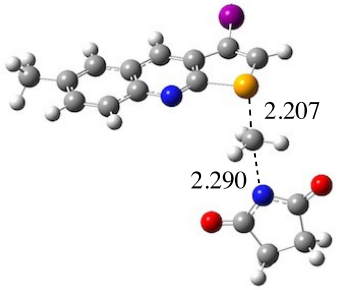
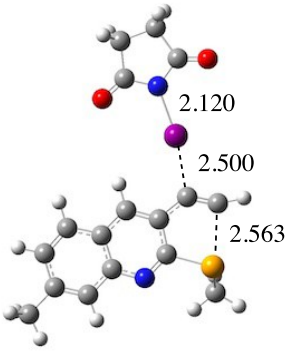
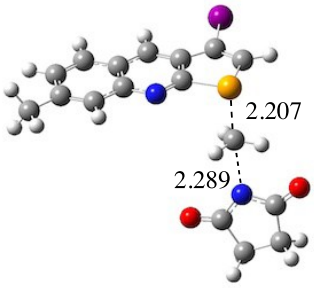
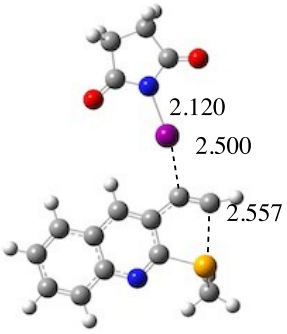
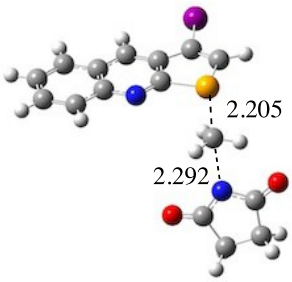
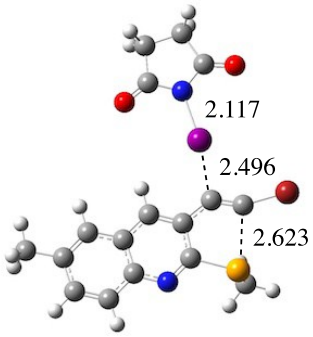
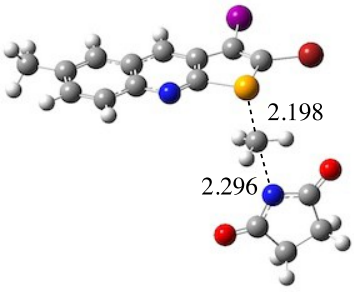
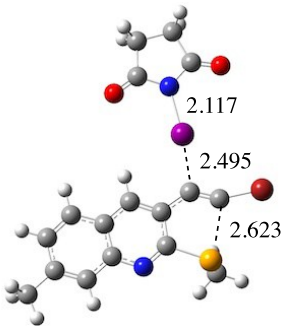
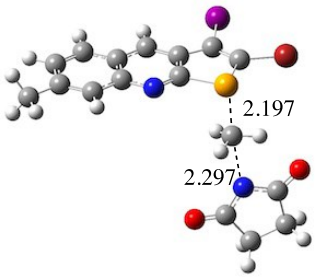
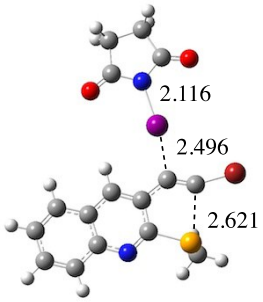
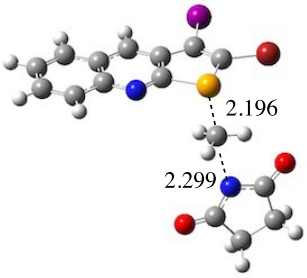
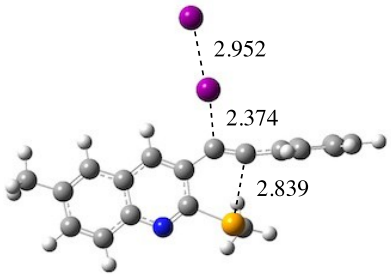
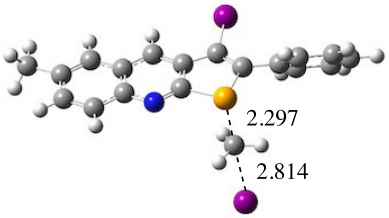
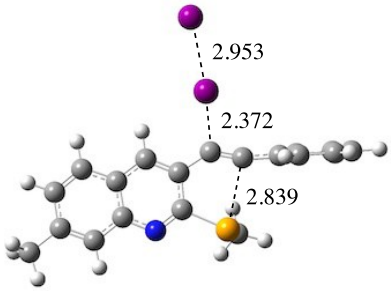
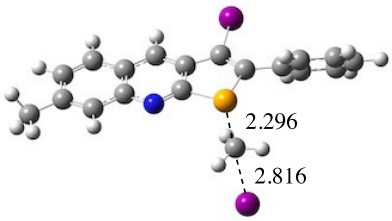
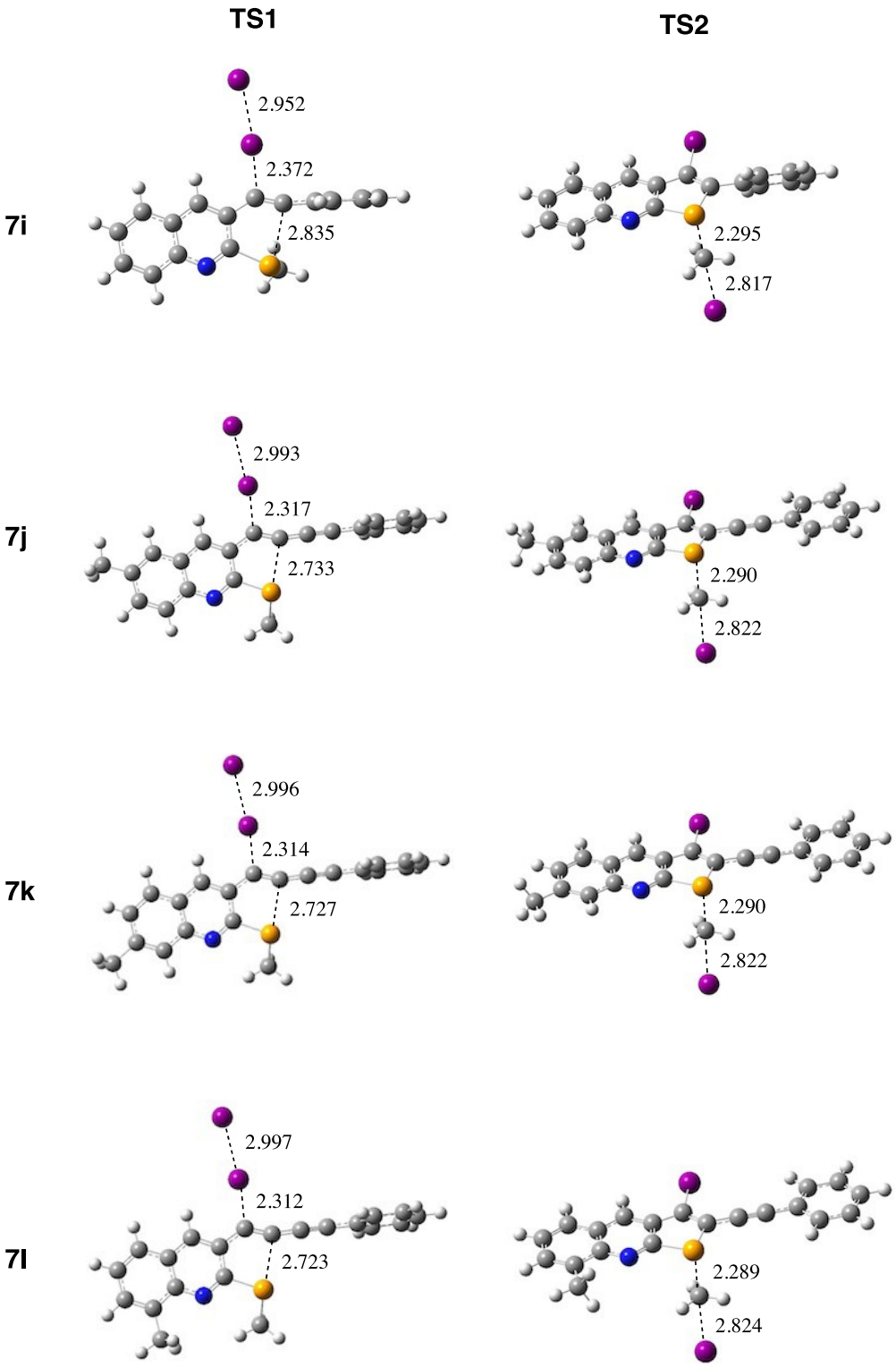


Figure S11. Relative Gibbs free energy profiles of the reactions leading to **7j**-**7m**.

	TS1	TS2
7a		
7b		
7c		
7d		

	TS1	TS2
7e		
7f		
7g		
7h		


TS1
TS2
7i
2.952
2.372
2.835
2.295
2.817
7j
2.993
2.317
2.733
2.290
2.822
7k
2.996
2.314
2.727
2.290
2.822
7l
2.997
2.312
2.723
2.289
2.824

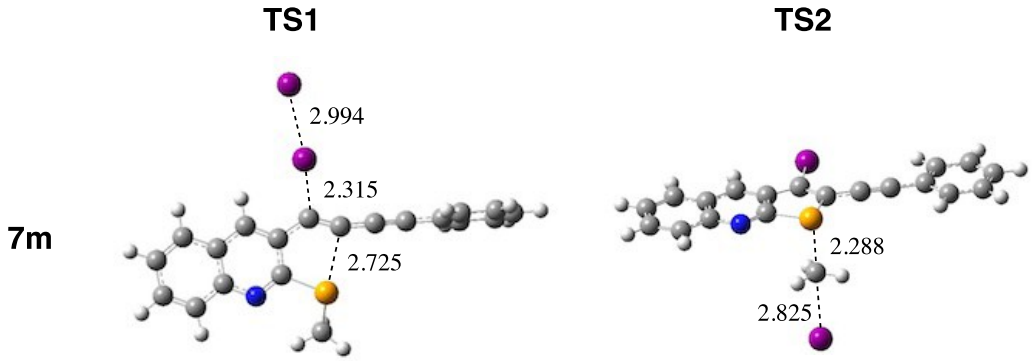


Figure S12. M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi!-optimized geometries (parameters are in [Å]) of **TS1** and **TS2** of the reactions leading to **7a**-**7m**.

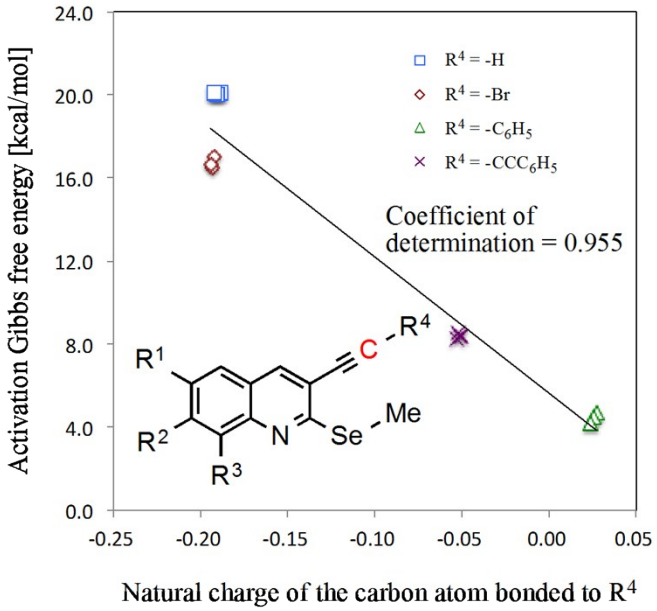


Figure S13. Relationship between natural charge of the carbon atom bonded to R^4 group (red-marked) and ΔG^a values of selenium-containing systems.

DFT-optimized cartesian coordinates [Å] and energies [hartree] of all the stationary points in the reactions of X = S.

I_2:

Atom	x	y	z
I	0.000000	0.000000	0.000000
I	0.000000	0.000000	2.687695

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.000513 hartree
Thermal correction to Gibbs free energy = -0.025205 hartree
M06-2X/Midi! electronic energy = -13780.9633469 hartree

I anion:

Atom	x	y	z
I	0.000000	0.000000	0.000000

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.000000 hartree
Thermal correction to Gibbs free energy = -0.016848 hartree
M06-2X/Midi! electronic energy = -6890.64389031 hartree

CH_3I:

Atom	x	y	z
C	0.000000	0.000000	0.000000
I	0.000000	0.000000	2.138908
H	1.033438	0.000000	-0.337075
H	-0.516719	-0.894984	-0.337075
H	-0.516719	0.894984	-0.337075

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.037382 hartree
Thermal correction to Gibbs free energy = 0.012704 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -6930.38193296 hartree

***N*-iodosuccinimide:**

Atom	x	y	z
C	0.691311	-1.312925	-0.000310
C	1.384163	0.928199	-0.000468
N	0.312149	0.031966	-0.000422
I	-1.617572	0.629634	-0.000557
C	2.209057	-1.356517	-0.000264

H	2.537253	-1.910972	-0.882215
H	2.537216	-1.910934	0.881724
C	2.661789	0.107638	-0.000293
H	3.245849	0.379866	-0.882233
H	3.245634	0.379945	0.881767
O	1.272137	2.127993	-0.000610
O	-0.078173	-2.240389	-0.000260

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.082495 hartree
Thermal correction to Gibbs free energy = 0.048186 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -7250.50798379 hartree

***N*-iodosuccinimide anion:**

Atom	x	y	z
C	0.682022	-1.240276	-0.000283
C	1.335639	0.873188	-0.000456
N	0.257178	0.048990	-0.000449
C	2.221006	-1.353565	-0.000253
H	2.539469	-1.919604	-0.880898
H	2.539442	-1.919566	0.880426
C	2.669873	0.098498	-0.000292
H	3.252232	0.385966	-0.880872
H	3.252051	0.386052	0.880382
O	1.306952	2.105847	-0.000596
O	-0.037480	-2.241658	-0.000293

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.080078 hartree
Thermal correction to Gibbs free energy = 0.050165 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -360.160648918 hartree

***N*-methylsuccinimide:**

Atom	x	y	z
C	0.757198	-1.441515	0.046455
C	1.271846	0.817594	-0.065973
N	0.274577	-0.142410	-0.016150
C	2.275428	-1.380290	0.042193
H	2.644969	-1.954951	-0.810025
H	2.645220	-1.862026	0.950159
C	2.615920	0.110851	-0.035881
H	3.173711	0.381123	-0.935335
H	3.182688	0.471778	0.825235
O	1.057277	2.007775	-0.123496
O	0.060009	-2.429709	0.095456

C	-1.134157	0.198736	-0.029414
H	-1.699641	-0.731235	0.018358
H	-1.372755	0.827512	0.830648
H	-1.377595	0.739287	-0.946213

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.121838 hartree
Thermal correction to Gibbs free energy = 0.089172 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -399.944724831 hartree

Reaction for 4a

Reactant1 of the reaction for 4a:

Atom	x	y	z	Atom	x	y	z
C	-2.223708	-2.662804	-1.211423	H	1.554119	0.350415	-1.739367
C	-2.460696	-1.523934	-0.487851	H	2.755436	4.381264	-0.559161
C	-1.497136	-0.483128	-0.464488	N	-1.753793	0.630959	0.279422
C	-0.296621	-0.645042	-1.201973	S	-1.320237	3.042473	1.261975
C	-0.081766	-1.837277	-1.940737	C	-0.812980	-4.112532	-2.731151
C	-1.021118	-2.839920	-1.954694	H	-0.838987	-4.981874	-2.066067
C	0.630962	0.419338	-1.170695	H	-1.605876	-4.248774	-3.473752
C	0.356965	1.555869	-0.440376	H	0.147292	-4.107475	-3.251466
C	-0.874731	1.598757	0.301492	H	-2.965061	-3.457674	-1.225118
C	2.061457	3.569587	-0.515760	C	0.009026	3.046891	2.507584
C	1.271147	2.658401	-0.465404	H	-0.219803	3.869297	3.187877
H	-3.374715	-1.387259	0.080700	H	0.981977	3.219969	2.047607
H	0.844042	-1.944310	-2.501119	H	0.008033	2.109924	3.065702

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.203413 hartree
Thermal correction to Gibbs free energy = 0.162621 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -954.796778124 hartree

Entrance1 of the reaction for 4a:

Atom	x	y	z	Atom	x	y	z
C	0.979473	-0.086319	-0.503897	H	3.325571	2.315694	0.087942
C	0.873851	-0.641088	0.744889	H	3.967650	2.274718	2.485097
C	1.660438	-0.137757	1.812168	H	4.437967	-0.976104	6.000360
C	2.542905	0.942058	1.560471	H	3.949995	-2.435516	5.079060
C	2.633647	1.493284	0.255886	H	3.620918	-2.325057	6.823302
C	1.867693	0.995282	-0.771079	N	7.042989	4.292986	2.131413
C	3.297120	1.436444	2.647011	C	6.371303	4.262075	0.912214
N	1.552508	-0.719468	3.041526	C	8.247181	4.998310	2.101073

C	3.167508	0.861056	3.893952	C	7.202714	5.040574	-0.091210
C	2.271125	-0.257535	4.030606	O	5.315181	3.703899	0.726504
C	3.878877	1.383167	5.025562	C	8.432425	5.521247	0.686780
C	4.470321	1.824474	5.984683	O	8.977580	5.141766	3.049282
H	4.960348	2.201005	6.857922	H	6.593232	5.856984	-0.485018
I	6.293756	3.371279	3.773103	H	7.448643	4.378059	-0.924025
S	2.030074	-1.052944	5.616658	H	8.519347	6.609105	0.729590
C	3.686520	-1.758561	5.892507	H	9.372796	5.128097	0.294279
H	0.375353	-0.475978	-1.319304	H	0.967981	1.942325	-2.482773
H	0.200842	-1.467234	0.949182	H	2.665867	2.379091	-2.219630
C	1.943797	1.561554	-2.163782	H	2.241016	0.790297	-2.881897

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.286877 hartree
Thermal correction to Gibbs free energy = 0.228085 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.31559179 hartree

TS1 of the reaction for 4a:

Atom	x	y	z	Atom	x	y	z
C	0.286528	-0.896887	0.026354	H	2.711339	1.387823	-0.671747
C	0.473015	-1.049918	1.375373	H	3.975407	1.953233	1.421584
C	1.488299	-0.317072	2.039174	H	4.093560	-2.014700	5.315868
C	2.302362	0.570312	1.285694	H	2.324361	-2.307634	5.250724
C	2.080371	0.704785	-0.108505	H	3.143210	-2.109255	6.828451
C	1.092243	-0.010118	-0.742953	N	7.262038	4.635571	1.967115
C	3.320500	1.279303	1.968180	C	7.085381	4.784567	0.603889
N	1.640003	-0.481383	3.387381	C	8.266871	5.437356	2.476939
C	3.483613	1.092956	3.317456	C	8.087406	5.813181	0.093077
C	2.582264	0.188545	3.981922	O	6.263699	4.188393	-0.059882
C	4.503889	1.683446	4.156534	C	8.874195	6.241413	1.332857
C	4.722743	1.460902	5.372402	O	8.596986	5.480015	3.642591
H	5.187306	1.565335	6.334280	H	7.537137	6.631366	-0.377462
I	6.083342	3.305869	3.129263	H	8.706067	5.345676	-0.676469
S	2.795755	-0.015729	5.751980	H	8.779076	7.304758	1.564529
C	3.131751	-1.801868	5.782655	H	9.940346	6.010234	1.273091
H	-0.493764	-1.461111	-0.477600	H	-0.177879	0.467195	-2.413452
H	-0.140945	-1.722660	1.964870	H	1.537013	0.829084	-2.679599
C	0.842973	0.121216	-2.221418	H	0.957253	-0.845843	-2.721812

Number of imaginary frequencies = 1 (-296.1152 cm^{-1})
Zero-point vibrational correction = 0.286209 hartree
Thermal correction to Gibbs free energy = 0.229343 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.28944455 hartree

IM of the reaction for 4a:

Atom	x	y	z	Atom	x	y	z
C	-0.069885	-1.185377	0.163265	H	2.297690	1.027105	-0.880473
C	0.200387	-1.224184	1.505788	H	3.683330	1.790792	1.055094
C	1.252674	-0.440152	2.037417	H	4.459595	-1.478132	4.902066
C	2.021028	0.383615	1.162095	H	2.911671	-2.083625	5.605525
C	1.707473	0.395914	-0.221322	H	4.178113	-1.410186	6.681833
C	0.683988	-0.369361	-0.727772	N	7.374698	4.674993	2.014326
C	3.078552	1.159578	1.701195	C	7.493067	4.876723	0.669331
N	1.495605	-0.494590	3.384687	C	8.245946	5.461249	2.711614
C	3.326668	1.090722	3.050044	C	8.577375	5.921797	0.372567
C	2.471916	0.239614	3.795643	O	6.836226	4.312819	-0.195973
C	4.355782	1.744211	3.860830	C	9.082435	6.321725	1.754455
C	4.305964	1.391802	5.155101	O	8.359635	5.491917	3.929827
H	4.914817	1.728401	5.983289	H	8.132331	6.746059	-0.191096
I	5.778530	3.118242	3.018298	H	9.343035	5.467646	-0.262166
S	2.951486	0.285542	5.538148	H	8.921979	7.376324	1.994058
C	3.721035	-1.357216	5.693979	H	10.141990	6.107042	1.917223
H	-0.878291	-1.788567	-0.240856	H	-0.690077	-0.037092	-2.348174
H	-0.372681	-1.843403	2.187455	H	1.003260	0.299123	-2.753156
C	0.342576	-0.365669	-2.193006	H	0.429678	-1.373005	-2.612616

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288864 hartree
Thermal correction to Gibbs free energy = 0.233426 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.32481211 hartree

Reactant2 of the reaction for 4a:

Atom	x	y	z	Atom	x	y	z
C	-2.390246	-2.707116	-1.629376	H	0.274561	4.676329	0.751974
C	-2.787346	-1.508017	-1.098908	N	-2.262133	0.712496	-0.373144
C	-1.837571	-0.478429	-0.898771	S	-1.724785	3.230465	0.478299
C	-0.473235	-0.705484	-1.254823	I	2.784128	2.941164	-0.457425
C	-0.104757	-1.960333	-1.802878	C	-0.659868	-4.291729	-2.568758
C	-1.035190	-2.954629	-1.992034	H	-0.886332	-5.093914	-1.859262
C	0.472410	0.328470	-1.044093	H	-1.232136	-4.492408	-3.479921
C	0.037390	1.511881	-0.501864	H	0.403536	-4.336210	-2.811597
C	-1.345616	1.600945	-0.209691	H	-3.121565	-3.495893	-1.782165
C	-0.005590	3.687681	0.415854	C	-2.019090	2.801809	2.224422
C	0.755149	2.730417	-0.137281	H	-1.194015	2.190881	2.588333
H	-3.818725	-1.316373	-0.824058	H	-2.107235	3.738285	2.774938
H	0.935282	-2.124310	-2.071836	H	-2.964197	2.256750	2.240622
H	1.517192	0.177525	-1.303429				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.207742 hartree
Thermal correction to Gibbs free energy = 0.164714 hartree

M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -7845.13564660 hartree

Entrance2 of the reaction for 4a:

Atom	x	y	z	Atom	x	y	z
C	-2.562580	-2.820484	-2.259158	H	2.372633	3.116605	-1.583491
C	-2.866930	-1.758805	-1.448979	H	-1.446778	2.147749	2.253727
C	-1.965129	-0.672787	-1.340410	H	-0.550721	1.529726	2.263320
C	-0.744994	-0.701677	-2.080752	H	-1.353637	3.011282	2.925170
C	-0.469265	-1.818885	-2.910264	H	-2.338753	1.568554	2.492150
C	-1.351714	-2.868046	-3.007931	N	-0.938120	1.127434	6.240363
C	0.154534	0.386364	-1.960667	C	-0.982213	3.174729	5.400998
N	-0.184331	1.425603	-1.131412	C	-1.065261	1.860194	5.098005
C	-1.432595	1.327991	-0.465933	C	-0.745087	2.020526	7.481917
C	-0.111611	3.434834	0.102068	O	0.197788	1.758253	7.970133
C	0.527136	2.650637	-0.778368	C	-1.548428	1.819276	8.196363
C	-3.256724	-3.652484	-2.339245	O	-0.771776	3.427177	6.903394
H	-3.787965	-1.718974	-0.877820	H	0.157521	3.985907	7.047604
I	0.461659	-1.832121	-3.470926	H	-1.587708	4.049727	7.281683
S	-1.070624	-4.060817	-3.880238	H	-1.061703	4.108890	4.590117
C	1.090907	0.387764	-2.512897	H	-0.968655	-0.098935	6.314671
H	0.194004	4.385055	0.517572	H	-1.864327	-4.192099	-4.622477
H	-2.300319	0.377255	-0.529157	H	-0.120120	-3.953344	-4.406671
C	-1.704421	2.788865	0.557278	H	-1.031571	-4.975847	-3.280609

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288764 hartree
Thermal correction to Gibbs free energy = 0.231668 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.31452027 hartree

TS2 of the reaction for 4a:

Atom	x	y	z	Atom	x	y	z
C	-2.573741	-2.807314	-1.584251	H	2.436120	3.105746	-1.718947
C	-2.885761	-1.623580	-0.971637	H	-1.397592	2.606382	2.294713
C	-1.969244	-0.542617	-1.007723	H	-0.416642	2.161050	2.193142
C	-0.724649	-0.710531	-1.686676	H	-1.473707	3.572625	2.782992
C	-0.440462	-1.954516	-2.309789	H	-2.239101	1.930951	2.387235
C	-1.337442	-2.993382	-2.269138	N	-0.833109	0.991330	5.244974
C	0.189207	0.368845	-1.712161	C	-1.155916	3.205803	5.281732
N	-0.161435	1.538993	-1.084438	C	-1.084635	2.102141	4.495557
C	-1.436386	1.576152	-0.458002	C	-0.717947	1.350112	6.736869
C	-0.115809	3.719814	-0.209051	O	0.264563	1.040170	7.103085
C	0.553975	2.795301	-0.917825	C	-1.468193	0.785858	7.297459
C	-3.280044	-3.632466	-1.552707	O	-0.937043	2.858668	6.761267
H	-3.825404	-1.479297	-0.449507	H	-0.081273	3.424625	7.139407
I	0.510026	-2.071058	-2.824049	H	-1.813946	3.169749	7.335628

S	-1.049439	-4.316535	-2.924608	H	-1.367864	4.350076	4.877921
C	1.147588	0.265029	-2.214807	H	-0.709919	-0.150288	4.816459
H	0.194116	4.723969	0.044924	H	-1.809666	-4.549127	-3.677222
H	-2.314119	0.627050	-0.392304	H	-0.072133	-4.313966	-3.411758
C	-1.710881	3.165521	0.311992	H	-1.064931	-5.124994	-2.186671

Number of imaginary frequencies = 1 (-491.5392 cm^{-1})
Zero-point vibrational correction = 0.288246 hartree
Thermal correction to Gibbs free energy = 0.232276 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.30495817 hartree

Product of the reaction for 4a:

Atom	x	y	z	Atom	x	y	z
C	-2.334102	-2.746097	-1.632118	H	0.952258	-2.102636	-2.242133
C	-2.712478	-1.569848	-1.047519	H	1.537358	0.194824	-1.450483
C	-1.769576	-0.519854	-0.865956	H	0.309641	4.622326	0.703893
C	-0.426077	-0.722732	-1.306845	N	-2.186810	0.632983	-0.279707
C	-0.074251	-1.962954	-1.911287	S	-1.643331	3.125830	0.605718
C	-0.995247	-2.964289	-2.078248	I	2.804906	2.977635	-0.638085
C	0.506830	0.318690	-1.125509	C	-0.635339	-4.279888	-2.714789
C	0.085943	1.487442	-0.531363	H	-0.818068	-5.109423	-2.023757
C	-1.285270	1.567575	-0.133688	H	-1.245185	-4.461055	-3.605993
C	0.012047	3.635590	0.375369	H	0.416451	-4.304236	-3.008442
C	0.791997	2.706785	-0.215421	H	-3.062635	-3.541685	-1.765423
H	-3.729136	-1.401979	-0.707645				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.168789 hartree
Thermal correction to Gibbs free energy = 0.128331 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -7805.45815953 hartree

Reaction for 4b

Reactant1 of the reaction for 4b:

Atom	x	y	z	Atom	x	y	z
C	-2.238411	-4.031314	-1.452622	H	0.594044	-0.274501	-2.803173
C	-2.329697	-3.017581	-0.528327	N	-1.705525	-0.853668	0.274465
C	-1.590051	-1.818353	-0.684343	S	-1.293603	1.484803	1.423200
C	-0.745862	-1.662381	-1.813527	H	-1.316359	-4.667723	-3.308268
C	-0.659071	-2.716054	-2.761059	C	-3.015756	-5.311195	-1.301110
C	-1.384754	-3.863030	-2.581001	H	-3.678284	-5.466147	-2.158926
C	-0.043539	-0.445373	-1.940237	H	-2.340366	-6.171681	-1.254085
C	-0.184921	0.538446	-0.984355	H	-3.624009	-5.301302	-0.394197

C	-1.035453	0.261369	0.141655	H	1.536866	3.783551	-1.487288
C	1.041282	2.849406	-1.332241	C	0.394215	1.649243	2.088373
C	0.475225	1.798289	-1.152617	H	0.316652	2.334272	2.934703
H	-2.967411	-3.108440	0.346138	H	1.073875	2.068369	1.346580
H	-0.012607	-2.595136	-3.625740	H	0.757476	0.683643	2.442059

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.203336 hartree
Thermal correction to Gibbs free energy = 0.162386 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -954.797102794 hartree

Entrance1 of the reaction for 4b:

Atom	x	y	z	Atom	x	y	z
C	0.961823	-0.087456	-0.522019	H	3.328776	2.323387	0.078635
C	0.874449	-0.629018	0.739217	H	3.976317	2.280476	2.488517
C	1.664480	-0.126454	1.803008	H	4.436405	-0.972025	6.003842
C	2.551261	0.952372	1.560814	H	3.960756	-2.427073	5.069320
C	2.638602	1.502543	0.254543	H	3.619919	-2.330293	6.811983
C	1.863038	0.992219	-0.752403	N	7.044741	4.291094	2.136288
C	3.304760	1.442493	2.647662	C	6.368939	4.258592	0.919505
N	1.555927	-0.711935	3.031648	C	8.248552	4.996974	2.101037
C	3.173115	0.863410	3.893356	C	7.196090	5.036904	-0.087495
C	2.275145	-0.254236	4.022443	O	5.312507	3.699421	0.738023
C	3.881549	1.382208	5.027990	C	8.428870	5.517986	0.685400
C	4.470568	1.821775	5.989475	O	8.982038	5.141890	3.046610
H	4.958243	2.197078	6.864519	H	6.584798	5.853201	-0.478773
I	6.301154	3.370755	3.781295	H	7.438606	4.374408	-0.921317
S	2.030991	-1.057504	5.604437	H	8.516733	6.605833	0.726350
C	3.689139	-1.756894	5.885693	H	9.367521	5.123583	0.290017
H	1.928003	1.411645	-1.752883	H	-0.512100	-1.431628	-1.343671
H	0.202546	-1.455140	0.952378	H	-0.501924	0.183518	-2.075780
C	0.131126	-0.609090	-1.663589	H	0.771092	-0.967776	-2.476436

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.286869 hartree
Thermal correction to Gibbs free energy = 0.228186 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.31594522 hartree

TS1 of the reaction for 4b:

Atom	x	y	z	Atom	x	y	z
C	0.272335	-0.918993	0.019608	H	2.707380	1.384288	-0.687570
C	0.482809	-1.053225	1.372173	H	3.984553	1.958954	1.413240
C	1.498528	-0.316284	2.028720	H	4.057545	-2.042740	5.320800
C	2.313963	0.574426	1.280002	H	2.281785	-2.290288	5.245994
C	2.084644	0.703725	-0.114391	H	3.096312	-2.107477	6.828244

C	1.093940	-0.022084	-0.720860	N	7.269739	4.643263	1.967313
C	3.330918	1.284090	1.960287	C	7.094353	4.793746	0.604198
N	1.652110	-0.479980	3.377899	C	8.272978	5.445677	2.478992
C	3.495329	1.096976	3.309848	C	8.095454	5.824389	0.095512
C	2.594166	0.191261	3.971223	O	6.274165	4.197330	-0.061319
C	4.515643	1.685178	4.150112	C	8.880581	6.251952	1.336550
C	4.735041	1.455636	5.365135	O	8.601996	5.487465	3.645047
H	5.200532	1.557456	6.326857	H	7.544482	6.642483	-0.374372
I	6.091051	3.309667	3.127024	H	8.715367	5.358769	-0.674172
S	2.807673	-0.010353	5.741761	H	8.784097	7.314900	1.569487
C	3.098876	-1.804016	5.781299	H	9.947045	6.022012	1.277515
H	0.923584	0.081272	-1.789026	H	-1.350079	-2.340427	-0.003802
H	-0.124090	-1.724451	1.972480	H	-1.517701	-1.014790	-1.169711
C	-0.803108	-1.693679	-0.693059	H	-0.372144	-2.317164	-1.483133

Number of imaginary frequencies = 1 (-296.3896 cm^{-1})
Zero-point vibrational correction = 0.286184 hartree
Thermal correction to Gibbs free energy = 0.229379 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.28969636 hartree

IM of the reaction for 4b:

Atom	x	y	z	Atom	x	y	z
C	-0.088583	-1.206002	0.157085	H	2.288951	1.025404	-0.894946
C	0.203816	-1.225106	1.500813	H	3.686270	1.797952	1.049109
C	1.254779	-0.437150	2.026056	H	4.456540	-1.474749	4.893687
C	2.026276	0.390216	1.156440	H	2.905347	-2.079869	5.590240
C	1.707199	0.397336	-0.227099	H	4.169603	-1.411888	6.672744
C	0.684054	-0.376621	-0.705257	N	7.380685	4.679275	2.017995
C	3.081488	1.166275	1.694816	C	7.502222	4.879941	0.673158
N	1.497528	-0.490629	3.374816	C	8.250729	5.465640	2.716605
C	3.328712	1.097181	3.044681	C	8.587742	5.924231	0.377984
C	2.472528	0.245020	3.786144	O	6.847266	4.315503	-0.193260
C	4.356326	1.749063	3.857768	C	9.089505	6.325334	1.760725
C	4.304719	1.395198	5.151755	O	8.361795	5.497177	3.935059
H	4.911997	1.731080	5.981340	H	8.144549	6.748083	-0.187727
I	5.781188	3.122511	3.018705	H	9.354820	5.469011	-0.254282
S	2.949227	0.289331	5.530498	H	8.928401	7.380136	1.999034
C	3.715687	-1.355146	5.683666	H	10.148670	6.110855	1.926257
H	0.448248	-0.364585	-1.765746	H	-0.811750	-2.733942	-1.170527
H	-0.362047	-1.841991	2.192157	H	-1.711059	-2.613135	0.353658
C	-1.200834	-2.037217	-0.421001	H	-1.937686	-1.400814	-0.921402

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288840 hartree
Thermal correction to Gibbs free energy = 0.233366 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.32505297 hartree

Reactant2 of the reaction for 4b:

Atom	x	y	z	Atom	x	y	z
C	-2.379419	-4.176065	-1.602536	N	-2.360195	-0.834946	-0.117411
C	-2.727280	-3.084049	-0.841257	S	-1.995353	1.707587	0.751960
C	-1.963289	-1.896017	-0.889787	I	1.815713	2.375360	-1.759783
C	-0.814722	-1.820745	-1.735878	H	-0.964970	-4.959590	-3.044032
C	-0.473755	-2.957580	-2.514655	C	-3.178297	-5.449157	-1.567893
C	-1.233927	-4.093996	-2.445451	H	-3.570870	-5.682774	-2.562714
C	-0.054912	-0.627810	-1.766862	H	-2.547937	-6.290128	-1.261924
C	-0.453512	0.421310	-0.975179	H	-4.017400	-5.374278	-0.873725
C	-1.619065	0.213701	-0.198712	H	-0.326757	3.519247	0.448914
C	-0.532745	2.506949	0.130377	C	-1.538372	1.166402	2.429976
C	0.122698	1.745089	-0.759403	H	-0.535112	0.743092	2.409164
H	-3.593616	-3.104220	-0.187684	H	-1.597944	2.041048	3.077118
H	0.396999	-2.909077	-3.161102	H	-2.284886	0.424388	2.717071
H	0.824522	-0.552847	-2.401342				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.207866 hartree
Thermal correction to Gibbs free energy = 0.164939 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -7845.13603631 hartree

Entrance2 of the reaction for 4b:

Atom	x	y	z	Atom	x	y	z
C	-2.577855	-2.834978	-2.249730	I	2.372052	3.134807	-1.596914
C	-2.857751	-1.756186	-1.443906	C	-1.435436	2.144217	2.247017
C	-1.954964	-0.672112	-1.344384	H	-0.535756	1.531380	2.253192
C	-0.735475	-0.691957	-2.086765	H	-1.347142	3.005348	2.922146
C	-0.466321	-1.813332	-2.915094	H	-2.323889	1.558582	2.482996
C	-1.360497	-2.847036	-2.989592	C	-0.930602	1.118183	6.234191
C	0.161115	0.396309	-1.970804	C	-0.985438	3.166712	5.398537
C	-0.177924	1.435597	-1.140226	N	-1.056150	1.852178	5.092452
C	-1.423931	1.331791	-0.472556	C	-0.752411	2.010296	7.478655
C	-0.108482	3.443294	0.096033	H	0.189126	1.754069	7.972605
C	0.530066	2.662036	-0.787406	H	-1.558950	1.801725	8.187365
H	-1.145536	-3.701833	-3.624641	C	-0.785866	3.417812	6.902620
H	-3.774092	-1.707273	-0.864131	H	0.138519	3.982915	7.053401
H	0.458478	-1.835654	-3.483442	H	-1.608466	4.033791	7.277180
C	-3.523361	-3.998156	-2.368326	O	-1.067677	4.101854	4.589058
H	1.095712	0.399457	-2.526111	O	-0.952288	-0.108521	6.306012
H	0.194921	4.394071	0.511743	H	-4.409374	-3.855546	-1.746691
N	-2.289537	0.379106	-0.531734	H	-3.845112	-4.128131	-3.406598
S	-1.697899	2.791224	0.553625	H	-3.030865	-4.926610	-2.062186

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288726 hartree
Thermal correction to Gibbs free energy = 0.231437 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.31489081 hartree

TS2 of the reaction for 4b:

Atom	x	y	z	Atom	x	y	z
C	-2.586503	-2.823958	-1.574768	I	2.435478	3.120715	-1.716763
C	-2.877967	-1.624344	-0.971116	C	-1.401799	2.603261	2.289136
C	-1.959866	-0.546541	-1.009831	H	-0.417763	2.164502	2.188576
C	-0.711278	-0.706351	-1.684176	H	-1.484883	3.567933	2.779350
C	-0.428969	-1.954561	-2.302116	H	-2.239096	1.922203	2.378769
C	-1.338357	-2.974863	-2.247017	C	-0.826532	0.987053	5.237040
C	0.199215	0.373482	-1.710196	C	-1.163803	3.199268	5.277465
C	-0.156289	1.544356	-1.084989	N	-1.088332	2.096948	4.489809
C	-1.432641	1.575676	-0.462092	C	-0.708756	1.344835	6.728975
C	-0.121154	3.725984	-0.211217	H	0.277104	1.041181	7.091443
C	0.553394	2.803324	-0.918065	H	-1.453200	0.774809	7.291454
H	-1.113794	-3.925868	-2.721907	C	-0.937993	2.851838	6.755903
H	-3.816918	-1.469625	-0.448681	H	-0.084932	3.423157	7.132099
H	0.519246	-2.081094	-2.815892	H	-1.815213	3.156241	7.333356
C	-3.549733	-3.978629	-1.542978	O	-1.383936	4.342703	4.875658
H	1.158889	0.271160	-2.210771	O	-0.696844	-0.153175	4.806734
H	0.183882	4.731740	0.042191	H	-4.463529	-3.719391	-1.004597
N	-2.308319	0.624703	-0.396478	H	-3.820561	-4.283046	-2.559118
S	-1.714631	3.164721	0.307110	H	-3.094938	-4.846491	-1.054543

Number of imaginary frequencies = 1 (-490.9347 cm^{-1})
Zero-point vibrational correction = 0.288213 hartree
Thermal correction to Gibbs free energy = 0.232125 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.30535025 hartree

Product of the reaction for 4b:

Atom	x	y	z	Atom	x	y	z
C	-2.334537	-4.199954	-1.636067	H	0.351553	-2.892802	-3.312856
C	-2.646978	-3.123539	-0.845726	H	0.789801	-0.538989	-2.547754
C	-1.895721	-1.917465	-0.907431	N	-2.260110	-0.888799	-0.096419
C	-0.793529	-1.829926	-1.812479	S	-1.871078	1.631863	0.788914
C	-0.486249	-2.959079	-2.624414	I	1.769608	2.409829	-1.949385
C	-1.231014	-4.100973	-2.537345	H	-0.988128	-4.956898	-3.161245
C	-0.053767	-0.632602	-1.867625	C	-3.123148	-5.480456	-1.578805
C	-0.422040	0.409486	-1.045737	H	-3.559568	-5.710997	-2.556318
C	-1.543645	0.200960	-0.184166	H	-2.477315	-6.321853	-1.306709
C	-0.529951	2.469266	0.043974	H	-3.931846	-5.416976	-0.847545
C	0.127989	1.733528	-0.875699	H	-0.309573	3.484104	0.346506

H	-3.478920	-3.160533	-0.148544

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.168760 hartree
Thermal correction to Gibbs free energy = 0.128290 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -7805.45858702 hartree

Reaction for 4c

Reactant1 of the reaction for 4c:

Atom	x	y	z	Atom	x	y	z
C	-2.244518	-3.968134	-1.553985	N	-1.721253	-0.854051	0.252600
C	-2.364287	-3.006685	-0.576658	S	-1.308133	1.458014	1.454960
C	-1.616870	-1.799065	-0.725386	H	-1.348461	-4.576082	-3.429430
C	-0.782603	-1.614553	-1.859204	H	1.494350	3.830107	-1.428044
C	-0.689442	-2.633917	-2.841363	H	-2.805681	-4.893435	-1.455905
C	-1.410299	-3.788521	-2.685347	C	-3.245121	-3.193647	0.626497
C	-0.084821	-0.390933	-1.961532	H	-2.660467	-3.139427	1.549554
C	-0.217797	0.571246	-0.983864	H	-3.999515	-2.403609	0.684944
C	-1.056824	0.266267	0.142790	H	-3.750650	-4.160945	0.586510
C	1.001519	2.891809	-1.290039	C	0.384564	1.612649	2.110090
C	0.438882	1.835834	-1.129811	H	0.311798	2.277248	2.972974
H	-0.047998	-2.480765	-3.704299	H	1.056778	2.051570	1.372968
H	0.544114	-0.199563	-2.826528	H	0.754014	0.640276	2.437869

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.203680 hartree
Thermal correction to Gibbs free energy = 0.163115 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -954.797263048 hartree

Entrance1 of the reaction for 4c:

Atom	x	y	z	Atom	x	y	z
C	0.963864	-0.089576	-0.492876	H	3.385036	2.259964	0.067831
C	0.831870	-0.649058	0.757934	H	4.027217	2.214191	2.457907
C	1.653597	-0.142257	1.809305	H	4.429337	-1.000657	6.012621
C	2.566578	0.912166	1.550138	H	3.921355	-2.455676	5.095306
C	2.673554	1.458133	0.244833	H	3.587544	-2.332970	6.837696
C	1.880741	0.958930	-0.755581	N	7.049156	4.317503	2.126229
C	3.337159	1.394107	2.630718	C	6.403632	4.250354	0.894433
N	1.543098	-0.707634	3.046114	C	8.225479	5.068731	2.113289
C	3.199107	0.835355	3.883946	C	7.225352	5.050375	-0.099991
C	2.276470	-0.259234	4.030003	O	5.373101	3.651096	0.693693
C	3.923883	1.351572	5.009678	C	8.419396	5.585549	0.697880

C	4.524536	1.787385	5.965596	O	8.930086	5.249009	3.074682
H	5.024285	2.157449	6.836100	H	6.593408	5.838757	-0.514899
I	6.301298	3.383496	3.761485	H	7.513685	4.389599	-0.920486
S	2.021236	-1.041527	5.620540	H	8.463222	6.676326	0.731635
C	3.665774	-1.771245	5.904997	H	9.382156	5.225675	0.328301
H	0.347061	-0.464056	-1.305264	H	-0.685464	-2.033275	0.133906
H	1.948314	1.363678	-1.760206	H	0.384385	-2.648735	1.412987
C	-0.137103	-1.762799	1.038958	H	-0.855012	-1.470470	1.811026

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.287095 hartree
Thermal correction to Gibbs free energy = 0.228494 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.31605577 hartree

TS1 of the reaction for 4c:

Atom	x	y	z	Atom	x	y	z
C	0.293148	-0.898667	0.036620	H	2.713907	1.402060	-0.672835
C	0.468109	-1.069904	1.391289	H	3.977619	1.958802	1.416148
C	1.494929	-0.318868	2.036519	H	4.051685	-2.052558	5.322852
C	2.307563	0.574346	1.285160	H	2.273763	-2.285852	5.251260
C	2.088288	0.717388	-0.108304	H	3.092907	-2.110950	6.832271
C	1.097072	-0.008408	-0.716201	N	7.270211	4.644112	1.962247
C	3.326634	1.283670	1.966009	C	7.092869	4.795059	0.599377
N	1.657026	-0.477728	3.384392	C	8.273758	5.446820	2.472926
C	3.497848	1.097353	3.313944	C	8.092692	5.826497	0.089840
C	2.599240	0.191924	3.977563	O	6.272125	4.198432	-0.065186
C	4.522028	1.684529	4.150680	C	8.879311	6.253904	1.329990
C	4.744331	1.450778	5.364532	O	8.604372	5.488221	3.638531
H	5.213990	1.550407	6.324522	H	7.540600	6.644512	-0.378863
I	6.094231	3.309677	3.123149	H	8.711786	5.361610	-0.680942
S	2.818004	-0.010829	5.747265	H	8.782595	7.316696	1.563541
C	3.095898	-1.806721	5.785568	H	9.945812	6.024551	1.269368
H	-0.484912	-1.462423	-0.470343	H	-1.121502	-2.502207	1.556841
H	0.921234	0.093592	-1.781998	H	0.230811	-2.781396	2.674508
C	-0.382796	-2.012648	2.194995	H	-0.905812	-1.480651	2.995121

Number of imaginary frequencies = 1 (-295.5396 cm^{-1})
Zero-point vibrational correction = 0.286430 hartree
Thermal correction to Gibbs free energy = 0.229894 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.28980295 hartree

IM of the reaction for 4c:

Atom	x	y	z	Atom	x	y	z
C	-0.065255	-1.185355	0.168642	H	2.301709	1.039396	-0.883361
C	0.189546	-1.240174	1.520163	H	3.681496	1.795626	1.052994

C	1.251581	-0.440500	2.032786	H	4.462055	-1.475540	4.896412
C	2.021963	0.387983	1.160858	H	2.911887	-2.080272	5.595597
C	1.715014	0.407795	-0.223702	H	4.178143	-1.412624	6.675966
C	0.691040	-0.365950	-0.704117	N	7.379532	4.678901	2.014349
C	3.078781	1.164174	1.700849	C	7.499748	4.879083	0.669241
N	1.501497	-0.489436	3.379690	C	8.249902	5.465851	2.712018
C	3.330486	1.096768	3.048893	C	8.584612	5.923637	0.372863
C	2.476049	0.244796	3.791910	O	6.844028	4.314204	-0.196222
C	4.360255	1.749127	3.859497	C	9.087375	6.325511	1.755034
C	4.310763	1.394663	5.153276	O	8.362100	5.497595	3.930320
H	4.920125	1.729947	5.981633	H	8.140676	6.747093	-0.192833
I	5.783503	3.123141	3.017109	H	9.351344	5.468421	-0.259813
S	2.955739	0.288745	5.535713	H	8.925926	7.380320	1.993057
C	3.722580	-1.355715	5.687648	H	10.146798	6.111653	1.919701
H	-0.870625	-1.788192	-0.240809	H	-1.380924	-2.649809	1.902864
H	0.451521	-0.356085	-1.762150	H	0.033058	-2.829572	2.962364
C	-0.610032	-2.106075	2.452448	H	-1.091284	-1.503736	3.228585

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.289123 hartree
Thermal correction to Gibbs free energy = 0.234047 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.32507366 hartree

Reactant2 of the reaction for 4c:

Atom	x	y	z	Atom	x	y	z
C	-2.296963	-4.156281	-1.636178	S	-1.967934	1.631042	0.906039
C	-2.671023	-3.131222	-0.796632	I	1.663835	2.499925	-1.805494
C	-1.935202	-1.914116	-0.865038	H	-0.966500	-4.863697	-3.188170
C	-0.843882	-1.773475	-1.778555	H	-0.376912	3.504621	0.564639
C	-0.503950	-2.860904	-2.622443	H	-2.844447	-5.093384	-1.599522
C	-1.220663	-4.026624	-2.546885	C	-3.813299	-3.260866	0.170653
C	-0.124690	-0.552991	-1.811620	H	-3.473981	-3.104336	1.198763
C	-0.502594	0.456088	-0.961926	H	-4.582403	-2.509709	-0.031309
C	-1.610974	0.185973	-0.124319	H	-4.264540	-4.252068	0.098304
C	-0.573600	2.498764	0.220368	C	-1.372957	1.040048	2.523163
C	0.048144	1.789207	-0.734080	H	-2.079333	0.270040	2.837186
H	0.322911	-2.752405	-3.316904	H	-0.365526	0.642431	2.407631
H	0.711212	-0.429095	-2.495475	H	-1.400434	1.888839	3.206235
N	-2.310629	-0.889266	-0.036647				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.208136 hartree
Thermal correction to Gibbs free energy = 0.165620 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -7845.13578781 hartree

Entrance2 of the reaction for 4c:

Atom	x	y	z	Atom	x	y	z
C	-2.559967	-2.813170	-2.244681	I	2.380766	3.123327	-1.604266
C	-2.882158	-1.756425	-1.423763	C	-1.427957	2.151787	2.247023
C	-1.960823	-0.672771	-1.339053	H	-0.530143	1.536274	2.254518
C	-0.742505	-0.696302	-2.085976	H	-1.337976	3.013456	2.921251
C	-0.461967	-1.809597	-2.918597	H	-2.318279	1.568994	2.483122
C	-1.357220	-2.844294	-2.991614	C	-0.934940	1.120340	6.231822
C	0.156538	0.392698	-1.971179	C	-0.983497	3.170292	5.399161
C	-0.175107	1.433902	-1.141947	N	-1.055597	1.856345	5.090849
C	-1.419675	1.334778	-0.471815	C	-0.758597	2.010196	7.478157
C	-0.096799	3.442056	0.091863	H	0.181371	1.751822	7.973987
C	0.538354	2.658409	-0.791784	H	-1.567156	1.801678	8.184571
H	-3.248822	-3.649161	-2.322139	C	-0.788450	3.418701	6.904278
H	-1.149129	-3.700101	-3.624913	H	0.136042	3.982531	7.059051
H	0.463497	-1.824210	-3.485519	H	-1.611613	4.034955	7.277165
C	-4.156154	-1.716405	-0.628347	O	-1.061504	4.106765	4.590805
H	1.089568	0.391821	-2.529110	O	-0.959282	-0.106433	6.301570
H	0.210695	4.392125	0.506329	H	-4.742203	-2.621387	-0.799373
N	-2.285198	0.383029	-0.529580	H	-3.945435	-1.631351	0.441644
S	-1.688426	2.796754	0.552381	H	-4.761725	-0.848374	-0.905062

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288952 hartree
Thermal correction to Gibbs free energy = 0.231814 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.31480493 hartree

TS2 of the reaction for 4c:

Atom	x	y	z	Atom	x	y	z
C	-2.565606	-2.800820	-1.569814	I	2.441266	3.114320	-1.728651
C	-2.900318	-1.619609	-0.949921	C	-1.395327	2.608928	2.287084
C	-1.964791	-0.543651	-1.005276	H	-0.413359	2.165258	2.187916
C	-0.718648	-0.706504	-1.686155	H	-1.474062	3.573349	2.778565
C	-0.424552	-1.947740	-2.309335	H	-2.235977	1.931691	2.375014
C	-1.333314	-2.969940	-2.249634	C	-0.840925	0.985114	5.236256
C	0.193190	0.374492	-1.715044	C	-1.154888	3.200758	5.275874
C	-0.154457	1.546614	-1.090072	N	-1.088590	2.097787	4.488291
C	-1.428179	1.581703	-0.463206	C	-0.722966	1.341693	6.728460
C	-0.109788	3.727264	-0.215948	H	0.258538	1.027191	7.093477
C	0.560356	2.803312	-0.925227	H	-1.475093	0.779955	7.289062
H	-3.266078	-3.630292	-1.537067	C	-0.935705	2.851116	6.754767
H	-1.115389	-3.921562	-2.722781	H	-0.077043	3.413019	7.132403
H	0.523428	-2.065386	-2.825036	H	-1.810519	3.165315	7.330604
C	-4.203371	-1.434692	-0.224952	O	-1.363063	4.346301	4.873641
H	1.150451	0.268458	-2.219426	O	-0.722977	-0.156558	4.806377
H	0.199310	4.731887	0.037200	H	-4.804113	-2.344739	-0.278943

N	-2.302916	0.631170	-0.394607	H	-4.031941	-1.189019	0.827273
S	-1.704471	3.172056	0.305721	H	-4.776504	-0.608594	-0.656057

Number of imaginary frequencies = 1 (-490.4853 cm^{-1})
Zero-point vibrational correction = 0.288525 hartree
Thermal correction to Gibbs free energy = 0.232800 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8205.30533831 hartree

Product of the reaction for 4c:

Atom	x	y	z	Atom	x	y	z
C	-2.317105	-4.175828	-1.639631	H	0.736783	-0.517600	-2.603434
C	-2.643809	-3.138399	-0.802108	N	-2.219095	-0.905680	-0.054673
C	-1.885383	-1.926201	-0.888041	S	-1.808647	1.605632	0.850237
C	-0.815785	-1.823413	-1.831685	I	1.740798	2.424476	-1.994232
C	-0.521221	-2.930289	-2.676672	H	-1.036957	-4.925058	-3.221748
C	-1.257037	-4.078131	-2.580077	H	-0.264906	3.465348	0.379876
C	-0.081948	-0.621202	-1.894943	H	-2.885674	-5.099920	-1.582369
C	-0.420701	0.410030	-1.048346	C	-3.765189	-3.237346	0.193391
C	-1.510998	0.187838	-0.151716	H	-3.399252	-3.076872	1.211960
C	-0.494527	2.454360	0.071371	H	-4.522568	-2.470123	0.006268
C	0.133604	1.732498	-0.879736	H	-4.240161	-4.219524	0.141275
H	0.292303	-2.841304	-3.390743				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.169072 hartree
Thermal correction to Gibbs free energy = 0.128931 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -7805.45863410 hartree

Reaction for 4d

Reactant1 of the reaction for 4d:

Atom	x	y	z	Atom	x	y	z
C	-2.327152	-2.621428	-1.397729	H	-3.569271	-1.408835	-0.123280
C	-2.618452	-1.518554	-0.634208	H	0.828044	-1.825316	-2.430034
C	-1.663070	-0.481297	-0.492162	H	-0.864500	-3.618053	-2.650585
C	-0.409760	-0.596543	-1.148409	H	1.466070	0.435580	-1.500071
C	-0.133704	-1.746961	-1.931125	H	2.539079	4.410050	-0.033924
C	-1.074698	-2.738050	-2.051658	N	-1.979931	0.592716	0.289268
C	0.504601	0.469875	-0.995381	S	-1.640482	2.949427	1.423826
C	0.169634	1.564599	-0.229113	C	-0.396705	2.907085	2.754165
C	-1.113216	1.561074	0.424570	H	-0.686584	3.688402	3.459152
C	1.852857	3.591963	-0.080784	H	0.601372	3.119204	2.370985
C	1.071599	2.673175	-0.133052	H	-0.417958	1.941894	3.261404

H	-3.059454	-3.415179	-1.504947

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.175616 hartree
Thermal correction to Gibbs free energy = 0.136942 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -915.489014844 hartree

Entrance1 of the reaction for 4d:

Atom	x	y	z	Atom	x	y	z
C	0.981115	-0.076786	-0.511559	H	1.941524	1.416841	-1.754772
C	0.875993	-0.631675	0.740067	H	3.339743	2.324760	0.089465
C	1.664781	-0.129136	1.804665	H	3.976930	2.278022	2.492026
C	2.552228	0.949906	1.560345	H	4.432633	-0.973064	6.007595
C	2.647070	1.504524	0.257710	H	3.956695	-2.429839	5.075731
C	1.873751	0.997388	-0.756414	H	3.614768	-2.329089	6.817949
C	3.305253	1.439970	2.650486	N	7.040733	4.289029	2.134004
N	1.554858	-0.714178	3.033934	C	6.359931	4.255474	0.920139
C	3.171875	0.861535	3.894724	C	8.245824	4.992653	2.092511
C	2.272804	-0.257126	4.024680	C	7.183702	5.031284	-0.091435
C	3.879024	1.380532	5.030255	O	5.302071	3.697212	0.744060
C	4.466385	1.820157	5.992523	C	8.420899	5.510992	0.675258
H	4.953444	2.195718	6.867846	O	8.983569	5.137521	3.034697
I	6.303068	3.371977	3.783202	H	6.571953	5.848266	-0.480598
S	2.027206	-1.058324	5.607094	H	7.421158	4.367604	-0.925772
C	3.685039	-1.757743	5.890486	H	8.511397	6.598695	0.713995
H	0.377480	-0.462825	-1.326661	H	9.356875	5.113785	0.276375
H	0.202556	-1.456464	0.947830				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.259126 hartree
Thermal correction to Gibbs free energy = 0.202938 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8166.00794528 hartree

TS1 of the reaction for 4d:

Atom	x	y	z	Atom	x	y	z
C	0.285059	-0.903033	0.025710	H	0.924415	0.090847	-1.791405
C	0.478546	-1.053509	1.376797	H	2.711738	1.391921	-0.678108
C	1.494828	-0.317650	2.033343	H	3.981452	1.957753	1.417428
C	2.309200	0.573369	1.282061	H	4.061361	-2.043884	5.318532
C	2.085476	0.709307	-0.111418	H	2.285884	-2.296362	5.250817
C	1.093782	-0.014446	-0.725067	H	3.106224	-2.111518	6.829735
C	3.327994	1.282759	1.964440	N	7.266072	4.640750	1.965501
N	1.649741	-0.482293	3.382793	C	7.088112	4.791168	0.602593
C	3.493019	1.094495	3.312379	C	8.270325	5.443170	2.475502
C	2.591691	0.187669	3.975600	C	8.088193	5.821895	0.092281

C	4.514313	1.682042	4.152134	O	6.266737	4.194602	-0.061216
C	4.733383	1.450522	5.366788	C	8.875700	6.249347	1.331885
H	5.200578	1.550757	6.327916	O	8.601327	5.484763	3.640934
I	6.089997	3.307870	3.126550	H	7.536273	6.640048	-0.376385
S	2.807904	-0.014934	5.745478	H	8.706656	5.356456	-0.678671
C	3.103842	-1.807965	5.782821	H	8.779751	7.312298	1.565011
H	-0.494360	-1.467188	-0.475860	H	9.942023	6.019308	1.270787
H	-0.130205	-1.725633	1.972156				

Number of imaginary frequencies = 1 (-295.5578 cm^{-1})
Zero-point vibrational correction = 0.258411 hartree
Thermal correction to Gibbs free energy = 0.203789 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8165.98146425 hartree

IM of the reaction for 4d:

Atom	x	y	z	Atom	x	y	z
C	-0.130579	-1.095939	0.129319	H	0.392028	-0.227621	-1.785573
C	0.158833	-1.171932	1.469233	H	2.276528	1.100355	-0.889594
C	1.232519	-0.420753	2.001130	H	3.689464	1.801797	1.056313
C	2.010111	0.413167	1.141999	H	4.454521	-1.553113	4.825767
C	1.683893	0.466370	-0.237229	H	2.981222	-2.160307	5.677040
C	0.637440	-0.272117	-0.729835	H	4.308494	-1.403386	6.617507
C	3.082254	1.161698	1.691114	N	7.363703	4.626424	2.002578
N	1.489831	-0.512171	3.345562	C	7.464461	4.844874	0.657791
C	3.340555	1.059096	3.035803	C	8.226029	5.421238	2.703527
C	2.480702	0.194510	3.763925	C	8.522858	5.916422	0.366156
C	4.382222	1.693347	3.843848	O	6.811585	4.275882	-0.206176
C	4.326573	1.312096	5.128711	C	9.034731	6.308422	1.748082
H	5.410817	1.789807	6.559929	O	8.349093	5.437366	3.920063
I	5.810111	3.076344	3.000793	H	8.052715	6.739014	-0.179421
S	2.961319	0.205958	5.507132	H	9.290487	5.488792	-0.284431
C	3.774844	-1.411882	5.665865	H	8.855957	7.356722	2.001968
H	-0.954888	-1.670707	-0.279844	H	10.099901	6.112433	1.897194
H	-0.416000	-1.794609	2.146193				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.261099 hartree
Thermal correction to Gibbs free energy = 0.207917 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8166.01649234 hartree

Reactant2 of the reaction for 4d:

Atom	x	y	z	Atom	x	y	z
C	-2.406507	-2.722651	-1.594187	H	-3.826641	-1.315558	-0.792477
C	-2.797486	-1.515860	-1.069053	H	0.928507	-2.146855	-2.043765
C	-1.842444	-0.491163	-0.877892	H	-0.769460	-3.915188	-2.363166

C	-0.476519	-0.717744	-1.231919	H	1.514772	0.163204	-1.284276
C	-0.108885	-1.975717	-1.773841	H	0.271468	4.673943	0.745811
C	-1.054536	-2.954221	-1.949152	N	-2.265270	0.705487	-0.358485
C	0.470104	0.316903	-1.026151	S	-1.728133	3.227781	0.477431
C	0.035843	1.502864	-0.490658	I	2.782485	2.931625	-0.450145
C	-1.348444	1.592913	-0.200443	C	-2.027531	2.807810	2.224952
C	-0.008478	3.683384	0.415128	H	-1.202634	2.200657	2.595416
C	0.753168	2.723199	-0.131663	H	-2.119390	3.747237	2.769775
H	-3.137877	-3.510007	-1.741408	H	-2.971776	2.261244	2.240624

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.180014 hartree
Thermal correction to Gibbs free energy = 0.139292 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -7805.82704795 hartree

Entrance2 of the reaction for 4d:

Atom	x	y	z	Atom	x	y	z
C	-2.565123	-2.824835	-2.251576	S	-1.701985	2.789891	0.554967
C	-2.864652	-1.757986	-1.441598	I	2.372988	3.124267	-1.589879
C	-1.960609	-0.674626	-1.340963	C	-1.442245	2.146018	2.250376
C	-0.740206	-0.698871	-2.083009	H	-0.544810	1.529985	2.258544
C	-0.464225	-1.816287	-2.912306	H	-1.350876	3.008978	2.922931
C	-1.357522	-2.854262	-2.992478	H	-2.333105	1.564621	2.487675
C	0.158254	0.390919	-1.964902	C	-0.932574	1.121814	6.233719
C	-0.180688	1.429469	-1.135994	C	-0.984137	3.170030	5.396998
C	-1.428909	1.328845	-0.468944	N	-1.059351	1.855552	5.091888
C	-0.110483	3.438061	0.098072	C	-0.748105	2.014183	7.477066
C	0.529000	2.655549	-0.783297	H	0.194792	1.756338	7.967589
H	-3.257367	-3.656416	-2.328340	H	-1.552370	1.807567	8.188914
H	-3.782315	-1.712937	-0.865634	C	-0.780640	3.421507	6.900449
H	0.463124	-1.833321	-3.476487	H	0.144824	3.985428	7.048945
H	-1.141679	-3.707360	-3.626519	H	-1.601605	4.038747	7.276554
H	1.093672	0.392865	-2.518748	O	-1.065520	4.104863	4.587005
H	0.193904	4.388719	0.513519	O	-0.957438	-0.104759	6.306202
N	-2.294900	0.377786	-0.529122				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.260994 hartree
Thermal correction to Gibbs free energy = 0.205978 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8166.00611423 hartree

TS2 of the reaction for 4d:

Atom	x	y	z	Atom	x	y	z
C	-2.573229	-2.813524	-1.577183	S	-1.714094	3.163863	0.309680
C	-2.883050	-1.624866	-0.966825	I	2.432014	3.115976	-1.724548

C	-1.965038	-0.546848	-1.008251	C	-1.399536	2.603437	2.290110
C	-0.718535	-0.709462	-1.687242	H	-0.417930	2.159307	2.189408
C	-0.431160	-1.953487	-2.308515	H	-1.476528	3.568677	2.780418
C	-1.338083	-2.979859	-2.254120	H	-2.239919	1.926623	2.383150
C	0.192998	0.372606	-1.714338	C	-0.835095	0.986211	5.243267
C	-0.160100	1.541708	-1.087825	C	-1.154354	3.201109	5.277940
C	-1.435857	1.574687	-0.460638	N	-1.085340	2.096621	4.492778
C	-0.120587	3.722336	-0.212568	C	-0.718413	1.346312	6.734727
C	0.551695	2.800144	-0.921828	H	0.263651	1.034778	7.100782
H	-3.277304	-3.638204	-1.543843	H	-1.469505	0.784135	7.296277
H	-3.820907	-1.475374	-0.443182	C	-0.934569	2.855303	6.757646
H	0.517263	-2.073031	-2.823383	H	-0.077230	3.419992	7.134141
H	-1.113787	-3.928627	-2.729582	H	-1.810176	3.168806	7.332656
H	1.151262	0.270116	-2.217484	O	-1.365117	4.345319	4.873181
H	0.186380	4.727511	0.041083	O	-0.714036	-0.156093	4.815943
N	-2.311124	0.624807	-0.393341				

Number of imaginary frequencies = 1 (-488.8679 cm^{-1})
Zero-point vibrational correction = 0.260470 hartree
Thermal correction to Gibbs free energy = 0.206620 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8165.99678305 hartree

Product of the reaction for 4d:

Atom	x	y	z	Atom	x	y	z
C	-2.419275	-2.699739	-1.600270	C	0.758605	2.739982	-0.216524
C	-2.807086	-1.468648	-1.142343	H	-3.160013	-3.476827	-1.758685
C	-1.844518	-0.443732	-0.931496	H	-3.845490	-1.238090	-0.928593
C	-0.468009	-0.718334	-1.202319	H	0.946689	-2.208403	-1.882556
C	-0.101312	-2.008522	-1.677907	H	-0.765410	-3.955634	-2.235068
C	-1.051867	-2.974149	-1.872225	H	1.534912	0.122321	-1.183555
C	0.480623	0.303412	-0.987338	H	0.251927	4.732432	0.504353
C	0.043994	1.524123	-0.526969	N	-2.276427	0.763697	-0.477283
C	-1.360453	1.676516	-0.295520	S	-1.736133	3.296425	0.283402
C	-0.045747	3.734150	0.212882	I	2.816566	2.910619	-0.414264

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.140927 hartree
Thermal correction to Gibbs free energy = 0.102608 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -7766.15046275 hartree

Reaction for 4e

Reactant1 of the reaction for 4e:

Atom	x	y	z	Atom	x	y	z
C	-2.127161	-2.722037	-1.194857	H	0.827028	-1.827218	-2.630931
C	-2.371950	-1.616328	-0.423637	H	1.480521	0.472536	-1.835477
C	-1.455433	-0.533821	-0.421389	Br	2.994762	5.100293	-0.530845
C	-0.292995	-0.619304	-1.229497	N	-1.717496	0.545396	0.370185
C	-0.068843	-1.778456	-2.016657	S	-1.336472	2.945522	1.400041
C	-0.962717	-2.822171	-2.009761	C	-0.743616	-4.060801	-2.836391
C	0.588723	0.483575	-1.215383	H	0.182349	-3.995291	-3.411889
C	0.307610	1.584641	-0.434192	H	-0.689611	-4.948967	-2.198382
C	-0.881815	1.550424	0.375299	H	-1.572697	-4.213592	-3.534941
C	1.908569	3.679387	-0.502734	C	0.060550	2.989207	2.568007
C	1.168204	2.724897	-0.462405	H	-0.183390	3.764912	3.296220
H	-2.832316	-3.549137	-1.191632	H	0.993044	3.247457	2.065931
H	-3.256798	-1.537898	0.199188	H	0.153813	2.032368	3.083028

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.194945 hartree
Thermal correction to Gibbs free energy = 0.150265 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -3516.24076679 hartree

Entrance1 of the reaction for 4e:

Atom	x	y	z	Atom	x	y	z
C	1.045697	0.066732	-0.561386	H	3.681211	2.126222	0.099280
C	0.832798	-0.466498	0.682941	H	4.259578	1.993942	2.529935
C	1.653624	-0.076934	1.772110	H	4.162905	-1.193300	6.102802
C	2.686086	0.869306	1.546014	H	3.577569	-2.593333	5.147934
C	2.882882	1.402621	0.245193	H	3.164944	-2.449017	6.871575
C	2.081242	1.015195	-0.801943	N	7.139556	4.485384	2.235127
C	3.472679	1.253031	2.654811	C	6.411904	4.143449	1.099921
N	1.429093	-0.637684	2.995658	C	8.195535	5.369553	1.987541
C	3.220253	0.703009	3.894743	C	7.025002	4.874023	-0.080134
C	2.175657	-0.276876	4.006048	O	5.463962	3.393487	1.091275
C	3.980650	1.149020	5.019411	C	8.196309	5.672688	0.499803
C	4.667024	1.590422	5.910167	O	8.945010	5.788362	2.832459
Br	5.734330	2.302995	7.159941	H	6.254815	5.502216	-0.533219
I	6.708697	3.766239	4.077666	H	7.329957	4.133775	-0.823110
S	1.783135	-1.019896	5.586282	H	8.092677	6.751803	0.367568
C	3.340619	-1.892408	5.949155	H	9.164872	5.378806	0.089388
H	0.413826	-0.235759	-1.392574	H	1.361454	2.073307	-2.534134
H	0.045999	-1.190337	0.868155	H	3.094226	2.281948	-2.223185
C	2.269244	1.566894	-2.190068	H	2.481842	0.763659	-2.903206

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.278033 hartree
Thermal correction to Gibbs free energy = 0.215730 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7587632 hartree

TS1 of the reaction for 4e:

Atom	x	y	z	Atom	x	y	z
C	0.197220	-0.932888	-0.040614	H	2.617219	1.368189	-0.703779
C	0.365416	-1.084842	1.310897	H	3.834325	1.954068	1.410950
C	1.366254	-0.345095	1.988536	H	4.558867	-1.373794	5.164975
C	2.185392	0.547535	1.247721	H	3.065371	-2.363164	5.264672
C	1.983335	0.680552	-0.149575	H	3.858844	-1.784025	6.756755
C	1.008723	-0.040812	-0.797740	N	7.213063	4.565828	2.014285
C	3.182609	1.268885	1.946753	C	7.060977	4.776825	0.656483
N	1.502873	-0.513392	3.338091	C	8.272537	5.268161	2.559074
C	3.323084	1.092187	3.300964	C	8.143016	5.743882	0.189861
C	2.426369	0.167916	3.949858	O	6.203657	4.268321	-0.034578
C	4.304951	1.735886	4.143371	C	8.944963	6.070533	1.450558
C	4.459410	1.596163	5.388182	O	8.598861	5.239240	3.726348
Br	5.265133	1.908383	6.958280	H	7.661451	6.615841	-0.258910
I	5.932938	3.282151	3.125330	H	8.734154	5.255789	-0.588576
S	2.612848	-0.041962	5.721043	H	8.918839	7.128562	1.721645
C	3.633339	-1.548622	5.715712	H	9.993770	5.770671	1.390203
H	-0.572036	-1.501747	-0.556091	H	-0.240805	0.429453	-2.485058
H	-0.251902	-1.761939	1.891796	H	1.475466	0.801620	-2.727860
C	0.779429	0.089558	-2.279408	H	0.906102	-0.876816	-2.778083

Number of imaginary frequencies = 1 (-303.2829 cm^{-1})
Zero-point vibrational correction = 0.276702 hartree
Thermal correction to Gibbs free energy = 0.216210 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7382529 hartree

IM of the reaction for 4e:

Atom	x	y	z	Atom	x	y	z
C	-0.091725	-1.106553	0.114039	H	2.272601	1.136359	-0.871556
C	0.186438	-1.189171	1.453011	H	3.666378	1.840494	1.079915
C	1.242709	-0.423564	2.002657	H	4.456506	-1.540216	4.831769
C	2.007154	0.427768	1.150716	H	2.994582	-2.163344	5.689937
C	1.685641	0.484928	-0.229527	H	4.317036	-1.389734	6.623564
C	0.658149	-0.262815	-0.754193	N	7.345232	4.634772	2.017103
C	3.066935	1.187240	1.708586	C	7.427081	4.845959	0.669857
N	1.493837	-0.520304	3.345917	C	8.234125	5.416421	2.699479
C	3.324745	1.076507	3.053409	C	8.502686	5.893477	0.354746
C	2.474073	0.197193	3.773539	O	6.747037	4.287761	-0.180123
C	4.362417	1.710763	3.867179	C	9.045208	6.281758	1.726114
C	4.307891	1.320001	5.149145	O	8.376403	5.437463	3.913913
Br	5.397836	1.779883	6.582700	H	8.042341	6.722718	-0.188873
I	5.789815	3.093001	3.027177	H	9.250923	5.445436	-0.304501
S	2.948526	0.203533	5.518050	H	8.893611	7.334761	1.977781

C	3.779157	-1.405953	5.674605	H	10.108211	6.063520	1.858361
H	-0.903375	-1.695229	-0.304647	H	-0.724874	0.123816	-2.354486
H	-0.383226	-1.829420	2.117870	H	0.966613	0.470606	-2.758613
C	0.308188	-0.211054	-2.216410	H	0.391133	-1.204406	-2.668924

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.278592 hartree
Thermal correction to Gibbs free energy = 0.220521 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7716842 hartree

Reactant2 of the reaction for 4e:

Atom	x	y	z	Atom	x	y	z
C	-2.360463	-2.794984	-1.587708	H	1.461426	0.215954	-1.456159
C	-2.759912	-1.623666	-0.999857	Br	0.388051	5.315500	1.055611
C	-1.833483	-0.566524	-0.839477	N	-2.259651	0.598090	-0.259184
C	-0.489804	-0.736868	-1.292504	S	-1.757368	3.121412	0.591734
C	-0.118654	-1.963952	-1.897950	I	2.705245	2.974102	-0.615221
C	-1.026806	-2.985063	-2.050242	C	-0.648946	-4.292124	-2.690664
C	0.433167	0.324437	-1.121139	H	0.397023	-4.294757	-3.003193
C	-0.001219	1.481017	-0.522462	H	-0.803922	-5.121356	-1.993169
C	-1.363840	1.512455	-0.135211	H	-1.273356	-4.484994	-3.568738
C	-0.053017	3.637467	0.424907	C	-1.882170	2.717525	2.361399
C	0.708513	2.711993	-0.188024	H	-1.022971	2.115220	2.653484
H	-3.073401	-3.605487	-1.710017	H	-1.916144	3.666294	2.898471
H	-3.775409	-1.475420	-0.649447	H	-2.819987	2.173163	2.480858
H	0.904917	-2.084772	-2.242164				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.197750 hartree
Thermal correction to Gibbs free energy = 0.152204 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10406.5805385 hartree

Entrance2 of the reaction for 4e:

Atom	x	y	z	Atom	x	y	z
C	-2.549602	-2.851779	-2.382045	I	2.370732	3.025064	-1.314333
C	-2.898815	-1.802179	-1.574155	C	-1.654995	2.108148	2.279492
C	-2.002221	-0.721382	-1.395669	H	-0.814511	1.417589	2.318422
C	-0.740827	-0.741476	-2.063402	H	-1.481484	2.991891	2.911467
C	-0.419271	-1.846085	-2.892923	H	-2.593862	1.620930	2.539529
C	-1.296897	-2.890884	-3.058886	C	-1.057545	1.179384	6.249206
C	0.152526	0.341797	-1.874195	C	-0.952377	3.191320	5.332285
C	-0.229455	1.369808	-1.048968	N	-1.230295	1.889188	5.098361
C	-1.514363	1.261442	-0.457167	C	-0.614101	2.077193	7.421020
C	-0.217557	3.354624	0.214363	H	0.341943	1.714575	7.809296
C	0.474853	2.580977	-0.640922	H	-1.345362	1.997126	8.230333

H	-3.239488	-3.680291	-2.516296	C	-0.540620	3.459227	6.789557
H	-3.851712	-1.768474	-1.057447	H	0.458674	3.903790	6.805144
H	0.542865	-1.853337	-3.398149	H	-1.227646	4.187643	7.229788
C	-0.967753	-4.070338	-3.932362	O	-1.009166	4.102898	4.494026
H	1.119243	0.348676	-2.370960	O	-1.225123	-0.031090	6.379082
Br	0.260480	4.927367	1.052434	H	-1.717223	-4.187125	-4.721559
N	-2.380112	0.316847	-0.588037	H	0.012037	-3.957394	-4.400757
S	-1.847975	2.710973	0.562947	H	-0.965939	-4.994940	-3.346265

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.278813 hartree
Thermal correction to Gibbs free energy = 0.220337 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7606154 hartree

TS2 of the reaction for 4e:

Atom	x	y	z	Atom	x	y	z
C	-2.512065	-2.865007	-1.844886	I	2.380110	3.121307	-1.470777
C	-2.873677	-1.721904	-1.184086	C	-1.527264	2.501512	2.365866
C	-1.980560	-0.622749	-1.128690	H	-0.649384	1.880433	2.242274
C	-0.708091	-0.727952	-1.766781	H	-1.390818	3.495070	2.785935
C	-0.372699	-1.930746	-2.442616	H	-2.463891	1.997270	2.565454
C	-1.247126	-2.988787	-2.490035	C	-1.059006	1.045418	5.435745
C	0.180721	0.370909	-1.702325	C	-0.921587	3.271027	5.248428
C	-0.217453	1.498737	-1.026539	N	-1.138443	2.107660	4.584394
C	-1.514492	1.471853	-0.445007	C	-0.750612	1.512483	6.869310
C	-0.251228	3.627767	-0.048959	H	0.175496	1.039033	7.206429
C	0.473339	2.755010	-0.776024	H	-1.550644	1.174389	7.533476
H	-3.200017	-3.705163	-1.883731	C	-0.656258	3.028552	6.740794
H	-3.835144	-1.624495	-0.691704	H	0.324802	3.435268	7.001027
H	0.598514	-2.000169	-2.925734	H	-1.401407	3.570479	7.329579
C	-0.905206	-4.269673	-3.201100	O	-0.932464	4.391204	4.735406
H	1.157296	0.315178	-2.176329	O	-1.208117	-0.132052	5.130385
Br	0.209414	5.313319	0.559962	H	-1.631276	-4.477508	-3.993605
N	-2.373454	0.505525	-0.466277	H	0.089531	-4.222676	-3.648996
S	-1.859489	3.017461	0.384497	H	-0.931336	-5.115558	-2.506680

Number of imaginary frequencies = 1 (-484.2193 cm^{-1})
Zero-point vibrational correction = 0.277875 hartree
Thermal correction to Gibbs free energy = 0.217190 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7519167 hartree

Product of the reaction for 4e:

Atom	x	y	z	Atom	x	y	z
C	-2.307146	-2.822249	-1.568990	H	-3.685308	-1.515119	-0.568137
C	-2.683475	-1.657483	-0.959625	H	0.928185	-2.097769	-2.339753

C	-1.757630	-0.587224	-0.821366	H	1.497733	0.209840	-1.567141
C	-0.434020	-0.755444	-1.329777	Br	0.462596	5.310365	0.896511
C	-0.083393	-1.983861	-1.957255	N	-2.171001	0.555022	-0.209399
C	-0.988201	-3.006311	-2.083031	S	-1.649198	3.055155	0.657140
C	0.482237	0.307911	-1.190954	I	2.741126	2.997560	-0.826270
C	0.064478	1.464621	-0.572098	C	-0.630218	-4.309577	-2.745432
C	-1.286267	1.508073	-0.106363	H	0.407927	-4.310464	-3.084929
C	-0.012993	3.600030	0.342227	H	-0.766518	-5.147742	-2.054194
C	0.766772	2.696215	-0.293071	H	-1.274723	-4.495766	-3.610876
H	-3.022480	-3.634378	-1.669689				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.158589 hartree
Thermal correction to Gibbs free energy = 0.115166 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10366.9052576 hartree

Reaction for 4f

Reactant1 of the reaction for 4f:

Atom	x	y	z	Atom	x	y	z
C	-2.243221	-4.025638	-1.419187	H	0.610575	-0.275938	-2.744033
C	-2.362619	-3.000095	-0.511052	N	-1.767270	-0.823669	0.279453
C	-1.624080	-1.799817	-0.663521	S	-1.393173	1.530167	1.408865
C	-0.751786	-1.654532	-1.772682	H	-1.271337	-4.681582	-3.242255
C	-0.636678	-2.719924	-2.704115	C	-3.018064	-5.307197	-1.269936
C	-1.361835	-3.867979	-2.527625	H	-3.656715	-5.478093	-2.142708
C	-0.049401	-0.437476	-1.896490	H	-2.339963	-6.163351	-1.192260
C	-0.218059	0.557546	-0.955944	H	-3.650343	-5.287408	-0.379737
C	-1.097297	0.291394	0.151339	Br	1.860941	4.432949	-1.457934
C	1.015007	2.868329	-1.264080	C	0.275572	1.718784	2.114636
C	0.445152	1.813459	-1.110894	H	0.164743	2.395740	2.963756
H	-3.022034	-3.082430	0.347861	H	0.967777	2.154929	1.394443
H	0.031058	-2.607452	-3.553463	H	0.646929	0.757103	2.470674

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.194869 hartree
Thermal correction to Gibbs free energy = 0.150061 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -3516.24112312 hartree

Entrance1 of the reaction for 4f:

Atom	x	y	z	Atom	x	y	z
C	1.033463	0.059399	-0.581293	H	3.697916	2.116355	0.085952
C	0.836495	-0.458872	0.677171	H	4.277554	1.985875	2.530324

C	1.661069	-0.070667	1.762828	H	4.151422	-1.184583	6.120317
C	2.701420	0.869175	1.544675	H	3.582500	-2.583019	5.153357
C	2.898334	1.397544	0.240891	H	3.148541	-2.446651	6.872224
C	2.084631	0.999363	-0.786363	N	7.137596	4.484741	2.234772
C	3.486981	1.248651	2.653548	C	6.416172	4.137489	1.097288
N	1.431931	-0.630649	2.986945	C	8.187473	5.377188	1.990624
C	3.228671	0.699836	3.893429	C	7.027180	4.873005	-0.080712
C	2.178845	-0.274377	3.998925	O	5.474004	3.380205	1.085562
C	3.986499	1.144009	5.020249	C	8.189971	5.681240	0.503096
C	4.671756	1.585459	5.911925	O	8.931303	5.801216	2.837904
Br	5.737769	2.298253	7.162833	H	6.253410	5.494758	-0.536555
I	6.706656	3.762172	4.075942	H	7.340698	4.135164	-0.822513
S	1.776695	-1.018628	5.576347	H	8.077368	6.759525	0.371335
C	3.333520	-1.885822	5.954186	H	9.162202	5.396093	0.095228
H	2.234181	1.403251	-1.784262	H	0.770919	-0.789671	-2.541355
H	0.047468	-1.179161	0.872451	H	-0.593692	-1.065286	-1.442830
C	0.167285	-0.342428	-1.744748	H	-0.336941	0.530462	-2.172318

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.278001 hartree
Thermal correction to Gibbs free energy = 0.215339 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7591269 hartree

TS1 of the reaction for 4f:

Atom	x	y	z	Atom	x	y	z
C	0.178568	-0.950958	-0.049252	H	2.617376	1.360118	-0.720042
C	0.367251	-1.082204	1.306833	H	3.843530	1.956279	1.404653
C	1.369421	-0.340309	1.978031	H	4.550529	-1.378486	5.160589
C	2.193934	0.552073	1.242473	H	3.050203	-2.358389	5.252242
C	1.988233	0.677945	-0.155928	H	3.842139	-1.788538	6.748770
C	1.010085	-0.052702	-0.776978	N	7.219397	4.570058	2.016375
C	3.190163	1.272639	1.940502	C	7.070263	4.780278	0.658176
N	1.504755	-0.506618	3.329219	C	8.276012	5.274810	2.563473
C	3.328411	1.097051	3.295665	C	8.151433	5.749424	0.193809
C	2.428352	0.174462	3.941038	O	6.215656	4.269867	-0.034890
C	4.309656	1.738547	4.139978	C	8.949922	6.077764	1.456251
C	4.462694	1.597360	5.384893	O	8.599303	5.247338	3.731653
Br	5.266516	1.907148	6.956517	H	7.669080	6.620412	-0.256013
I	5.938257	3.284709	3.125238	H	8.745218	5.262522	-0.583351
S	2.611134	-0.035766	5.713329	H	8.921698	7.135860	1.726857
C	3.621967	-1.548892	5.707583	H	9.999288	5.779335	1.398476
H	0.857342	0.048217	-1.848073	H	-1.438706	-2.377268	-0.097261
H	-0.246446	-1.754869	1.898511	H	-1.591478	-1.053560	-1.267347
C	-0.882635	-1.729751	-0.778447	H	-0.437035	-2.352861	-1.560627

Number of imaginary frequencies = 1 (-303.2063 cm^{-1})

Zero-point vibrational correction = 0.276686 hartree
Thermal correction to Gibbs free energy = 0.216129 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7384138 hartree

IM of the reaction for 4f:

Atom	x	y	z	Atom	x	y	z
C	-0.109157	-1.125354	-1.125354	H	2.266189	1.136383	1.136383
C	0.190565	-1.188937	-1.188937	H	3.670831	1.848160	1.848160
C	1.245372	-0.419550	-0.419550	H	4.452584	-1.537417	-1.537417
C	2.013549	0.435276	0.435276	H	2.986139	-2.160383	-2.160383
C	1.687170	0.487811	0.487811	H	4.306832	-1.392676	-1.392676
C	0.660238	-0.269094	-0.269094	N	7.350429	4.638106	4.638106
C	3.070982	1.194428	1.194428	C	7.433864	4.847814	4.847814
N	1.495785	-0.515857	-0.515857	C	8.238854	5.420159	5.420159
C	3.327296	1.082966	1.082966	C	8.510165	5.894639	5.894639
C	2.474640	0.202759	0.202759	O	6.754560	4.288959	4.288959
C	4.363392	1.715130	1.715130	C	9.051608	6.283894	6.283894
C	4.306497	1.322561	1.322561	O	8.379673	5.442668	5.442668
Br	5.393593	1.779798	1.779798	H	8.050525	6.723594	6.723594
I	5.792868	3.096795	3.096795	H	9.258774	5.445834	5.445834
S	2.945503	0.206983	0.206983	H	8.900769	7.337291	7.337291
C	3.772403	-1.404627	-1.404627	H	10.114281	6.064791	6.064791
H	0.418875	-0.222024	-0.222024	H	-1.729033	-2.540406	-2.540406
H	-0.372176	-1.827326	-1.827326	H	-1.968058	-1.280307	-1.280307
C	-1.226237	-1.934913	-1.934913	H	-0.843816	-2.601984	-2.601984

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.278588 hartree
Thermal correction to Gibbs free energy = 0.220479 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7718980 hartree

Reactant2 of the reaction for 4f:

Atom	x	y	z	Atom	x	y	z
C	-2.073934	-3.030823	-1.268374	N	-2.018786	0.283992	0.273395
C	-2.397968	-1.955991	-0.472772	S	-1.645351	2.814071	1.167279
C	-1.648025	-0.759939	-0.534412	I	2.070131	3.537429	-1.490097
C	-0.538934	-0.657171	-1.428793	C	-2.857571	-4.312862	-1.220595
C	-0.222842	-1.776102	-2.242910	H	-3.292971	-4.532883	-2.200544
C	-0.968585	-2.921317	-2.160276	H	-2.205447	-5.152267	-0.959293
C	0.207912	0.543586	-1.471502	H	-3.664606	-4.259519	-0.487508
C	-0.162662	1.575605	-0.643717	H	-0.718713	-3.773031	-2.786451
C	-1.290410	1.339369	0.179541	Br	0.161921	5.338754	1.112360
C	-0.208332	3.639009	0.493146	C	-1.082269	2.290381	2.816329
C	0.420172	2.897389	-0.438297	H	-0.098125	1.831842	2.729698
H	-3.233574	-1.996591	0.218727	H	-1.064890	3.181920	3.444243

H	0.617089	-1.707351	-2.927148	H	-1.830008	1.581811	3.175490
H	1.057163	0.638518	-2.143114				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.197618 hartree
Thermal correction to Gibbs free energy = 0.151631 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10406.5808408 hartree

Entrance2 of the reaction for 4f:

Atom	x	y	z	Atom	x	y	z
C	-2.563072	-2.876222	-2.295800	I	2.361285	3.083672	-1.508923
C	-2.864368	-1.802948	-1.490228	C	-1.514914	2.143101	2.258201
C	-1.967629	-0.716723	-1.365761	H	-0.645944	1.487737	2.277085
C	-0.732389	-0.727103	-2.081564	H	-1.372924	3.027830	2.895901
C	-0.441251	-1.842800	-2.909931	H	-2.427655	1.614535	2.530925
C	-1.329991	-2.879295	-3.009087	C	-0.992537	1.132006	6.212890
C	0.156847	0.364384	-1.941547	C	-0.964255	3.175079	5.361672
C	-0.201965	1.399035	-1.112659	N	-1.122734	1.864538	5.070874
C	-1.461031	1.283020	-0.470820	C	-0.711219	2.020597	7.440664
C	-0.163336	3.399075	0.126196	H	0.236351	1.716069	7.894152
C	0.503109	2.622707	-0.747450	H	-1.495088	1.860980	8.186531
H	-1.098280	-3.729672	-3.644204	C	-0.692757	3.424415	6.854625
H	-3.793072	-1.760356	-0.929955	H	0.264890	3.941321	6.964990
H	0.495487	-1.858758	-3.458530	H	-1.467106	4.084831	7.255479
C	-3.501127	-4.042363	-2.441275	O	-1.022959	4.107063	4.546773
H	1.102308	0.374347	-2.477732	O	-1.081543	-0.090888	6.296104
Br	0.326275	4.994619	0.914400	H	-4.402694	-3.904976	-1.841148
N	-2.322146	0.329301	-0.554905	H	-3.796735	-4.170084	-3.487558
S	-1.770229	2.740966	0.546906	H	-3.012821	-4.970007	-2.125982

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.278586 hartree
Thermal correction to Gibbs free energy = 0.218702 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7608816 hartree

TS2 of the reaction for 4f:

Atom	x	y	z	Atom	x	y	z
C	-2.530381	-2.882498	-1.852274	I	2.390104	3.120713	-1.445385
C	-2.870104	-1.723984	-1.195594	C	-1.533430	2.492358	2.365963
C	-1.972171	-0.630680	-1.136000	H	-0.648529	1.880645	2.245511
C	-0.694127	-0.729524	-1.764688	H	-1.409972	3.487262	2.786834
C	-0.362191	-1.935345	-2.439138	H	-2.465735	1.978232	2.560616
C	-1.253100	-2.972844	-2.478689	C	-1.033886	1.046431	5.437445
C	0.194297	0.366915	-1.694204	C	-0.947502	3.274290	5.247030
C	-0.207967	1.494707	-1.019310	N	-1.145855	2.105834	4.586075

C	-1.508294	1.464048	-0.446362	C	-0.727156	1.522026	6.868545
C	-0.251166	3.622953	-0.040686	H	0.210416	1.068546	7.201317
C	0.479170	2.751439	-0.763509	H	-1.516407	1.168324	7.537495
H	-0.990453	-3.891290	-2.996192	C	-0.665569	3.039533	6.737517
H	-3.832551	-1.614991	-0.705399	H	0.308959	3.466830	6.989228
H	0.608197	-2.016226	-2.919631	H	-1.416965	3.566803	7.331620
C	-3.470724	-4.053985	-1.925448	O	-0.984270	4.393304	4.732609
H	1.173472	0.311127	-2.162929	O	-1.155803	-0.134595	5.133896
Br	0.202646	5.308854	0.572703	H	-4.410368	-3.842309	-1.411345
N	-2.367759	0.498332	-0.473631	H	-3.694390	-4.304392	-2.967481
S	-1.860398	3.008666	0.383120	H	-3.018342	-4.940060	-1.468520

Number of imaginary frequencies = 1 (-484.5683 cm^{-1})
Zero-point vibrational correction = 0.277869 hartree
Thermal correction to Gibbs free energy = 0.217560 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7522541 hartree

Product of the reaction for 4f:

Atom	x	y	z	Atom	x	y	z
C	-2.035496	-3.042824	-1.300217	H	0.581050	-1.700094	-3.056698
C	-2.323871	-1.978017	-0.484435	H	1.041347	0.642777	-2.271939
C	-1.580528	-0.769056	-0.558296	N	-1.918533	0.249098	0.279177
C	-0.512200	-0.663880	-1.500401	S	-1.510659	2.754626	1.187836
C	-0.230372	-1.779554	-2.338807	I	2.046649	3.559272	-1.671788
C	-0.967179	-2.926131	-2.239995	C	-2.814959	-4.328189	-1.229731
C	0.222446	0.536966	-1.564390	H	-3.284553	-4.549989	-2.193722
C	-0.118592	1.566033	-0.715123	H	-2.155293	-5.168808	-0.990470
C	-1.208976	1.339550	0.180486	H	-3.597336	-4.277631	-0.469452
C	-0.190979	3.601837	0.403560	H	-0.743929	-3.772139	-2.884367
C	0.444192	2.886728	-0.552116	Br	0.186782	5.337947	0.953690
H	-3.129163	-2.028587	0.242427				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.158578 hartree
Thermal correction to Gibbs free energy = 0.115144 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10366.9056556 hartree

Reaction for 4g

Reactant1 of the reaction for 4g:

Atom	x	y	z	Atom	x	y	z
C	-2.282686	-2.605550	-1.343736	H	-3.407824	-1.390043	0.032297
C	-2.505040	-1.501409	-0.558796	H	0.772298	-1.815018	-2.646116

C	-1.539477	-0.465442	-0.500808	H	-0.935068	-3.605787	-2.716882
C	-0.348272	-0.583006	-1.263859	H	1.490055	0.445366	-1.781689
C	-0.142423	-1.734756	-2.066026	Br	3.132465	4.989160	-0.393297
C	-1.091553	-2.724810	-2.103345	N	-1.784477	0.609582	0.304397
C	0.577326	0.481854	-1.193909	S	-1.342894	2.967191	1.401650
C	0.311887	1.578615	-0.402653	C	0.020159	2.939271	2.609655
C	-0.908247	1.576625	0.362576	H	-0.219715	3.707718	3.346900
C	1.992328	3.611058	-0.394824	H	0.975352	3.176137	2.140985
C	1.214600	2.685934	-0.384554	H	0.065862	1.969590	3.106764
H	-3.022651	-3.398088	-1.386245				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.167159 hartree
Thermal correction to Gibbs free energy = 0.124728 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -3476.93311319 hartree

Entrance1 of the reaction for 4g:

Atom	x	y	z	Atom	x	y	z
C	1.045698	0.067837	-0.569545	H	2.234969	1.411267	-1.785823
C	0.832992	-0.462617	0.678875	H	3.697421	2.121870	0.094853
C	1.657446	-0.073465	1.764080	H	4.271996	1.987326	2.529901
C	2.696252	0.868751	1.542706	H	4.153483	-1.184844	6.119337
C	2.897481	1.402105	0.242861	H	3.584708	-2.583898	5.152973
C	2.085515	1.006119	-0.790347	H	3.152134	-2.447540	6.872156
C	3.482804	1.248691	2.653540	N	7.136375	4.483818	2.234259
N	1.430334	-0.634069	2.988858	C	6.410949	4.137889	1.099035
C	3.226462	0.699256	3.892004	C	8.187861	5.373550	1.986740
C	2.177153	-0.277601	3.999582	C	7.020442	4.871225	-0.081053
C	3.984672	1.143618	5.018646	O	5.466901	3.382849	1.090404
C	4.670099	1.584711	5.910257	C	8.187099	5.676597	0.499011
Br	5.735725	2.296683	7.161612	O	8.934947	5.796226	2.831786
I	6.708602	3.763435	4.076982	H	6.246983	5.494879	-0.534825
S	1.777847	-1.021129	5.577678	H	7.329783	4.132294	-0.823526
C	3.336017	-1.886729	5.953898	H	8.077159	6.755110	0.366828
H	0.413927	-0.231825	-1.399532	H	9.157397	5.388441	0.088673
H	0.044702	-1.183234	0.869555				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.250282 hartree
Thermal correction to Gibbs free energy = 0.190085 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10727.4512908 hartree

TS1 of the reaction for 4g:

Atom	x	y	z	Atom	x	y	z
C	0.194156	-0.935438	-0.042929	H	0.860059	0.059024	-1.849874

C	0.365691	-1.083098	1.311439	H	2.621342	1.371089	-0.709109
C	1.367312	-0.341157	1.983123	H	3.839781	1.958266	1.410380
C	2.189856	0.552810	1.245441	H	4.548936	-1.385150	5.161629
C	1.989647	0.685732	-0.151924	H	3.047181	-2.362819	5.256088
C	1.011792	-0.044008	-0.780636	H	3.842534	-1.793702	6.751090
C	3.187261	1.273620	1.945884	N	7.214829	4.568241	2.014671
N	1.504003	-0.508730	3.334549	C	7.058827	4.781456	0.657612
C	3.326556	1.096156	3.299342	C	8.276656	5.268680	2.557430
C	2.426981	0.171538	3.946092	C	8.140055	5.748595	0.189405
C	4.308705	1.736667	4.143481	O	6.199123	4.274517	-0.031614
C	4.461817	1.592315	5.388067	C	8.946322	6.072253	1.448140
Br	5.268214	1.899969	6.958790	O	8.606502	5.237359	3.723620
I	5.936922	3.283870	3.126578	H	7.657639	6.621783	-0.256051
S	2.612340	-0.039525	5.717829	H	8.728296	5.261650	-0.591933
C	3.621053	-1.554129	5.710173	H	8.922194	7.129840	1.721112
H	-0.573867	-1.503733	-0.557144	H	9.994609	5.771377	1.383915
H	-0.248986	-1.757721	1.897775				

Number of imaginary frequencies = 1 (-302.5052 cm^{-1})
Zero-point vibrational correction = 0.248917 hartree
Thermal correction to Gibbs free energy = 0.190691 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10727.4301111 hartree

IM of the reaction for 4g:

Atom	x	y	z	Atom	x	y	z
C	-0.096382	-1.109986	0.111588	H	0.419117	-0.216416	-1.793761
C	0.186521	-1.189015	1.452646	H	2.272108	1.140599	-0.878668
C	1.242692	-0.420773	1.995793	H	3.669588	1.845330	1.077713
C	2.009814	0.432913	1.146864	H	4.450412	-1.542820	4.825363
C	1.688816	0.490830	-0.233573	H	2.986270	-2.162621	5.682504
C	0.659648	-0.264292	-0.737171	H	4.310948	-1.394066	6.617251
C	3.069770	1.192069	1.706029	N	7.348098	4.634356	2.018842
N	1.494700	-0.517077	3.340915	C	7.429521	4.845266	0.671417
C	3.326709	1.080364	3.050288	C	8.236191	5.417145	2.701163
C	2.473827	0.200119	3.768371	C	8.503939	5.893838	0.356174
C	4.364293	1.712270	3.865623	O	6.749910	4.286095	-0.178173
C	4.308440	1.319487	5.146856	C	9.046135	6.283033	1.727448
Br	5.397840	1.776077	6.581754	O	8.378360	5.438453	3.915533
I	5.793755	3.094786	3.027046	H	8.042581	6.722460	-0.187529
S	2.947183	0.204515	5.514173	H	9.252634	5.446558	-0.303057
C	3.773212	-1.407656	5.668172	H	8.893400	7.335933	1.978833
H	-0.906260	-1.698519	-0.306164	H	10.109381	6.065980	1.859647
H	-0.378835	-1.827637	2.122532				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.250846 hartree

Thermal correction to Gibbs free energy = 0.195003 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10727.4632338 hartree

Reactant2 of the reaction for 4g:

Atom	x	y	z	Atom	x	y	z
C	-2.402571	-2.763277	-1.651432	H	-3.834411	-1.383836	-0.822693
C	-2.804116	-1.569263	-1.105126	H	0.925364	-2.146906	-2.100501
C	-1.858470	-0.538859	-0.900092	H	-0.755518	-3.926416	-2.443400
C	-0.491591	-0.744783	-1.262784	H	1.488680	0.159724	-1.316179
C	-0.112762	-1.990267	-1.824937	Br	0.382206	5.316226	1.061215
C	-1.049326	-2.975271	-2.013181	N	-2.289975	0.645264	-0.359384
C	0.444357	0.297715	-1.048556	S	-1.778808	3.162320	0.503022
C	0.001576	1.472725	-0.494983	I	2.739586	2.907723	-0.456703
C	-1.381944	1.538745	-0.192063	C	-2.003270	2.764830	2.264815
C	-0.056911	3.640172	0.425103	H	-1.201086	2.102814	2.588762
C	0.717860	2.692433	-0.134659	H	-1.991985	3.713159	2.803937
H	-3.126423	-3.555221	-1.810333	H	-2.981124	2.287776	2.343359

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.169949 hartree
Thermal correction to Gibbs free energy = 0.126427 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10367.2718139 hartree

Entrance2 of the reaction for 4g:

Atom	x	y	z	Atom	x	y	z
C	-2.552914	-2.862858	-2.298353	S	-1.773116	2.740841	0.549664
C	-2.872996	-1.801896	-1.488395	I	2.358264	3.078324	-1.509553
C	-1.975097	-0.716261	-1.363708	C	-1.516984	2.143485	2.261410
C	-0.740092	-0.730342	-2.081230	H	-0.649919	1.485640	2.279778
C	-0.442991	-1.841835	-2.910975	H	-1.371480	3.028837	2.897584
C	-1.330451	-2.882913	-3.014593	H	-2.431083	1.618172	2.535790
C	0.150776	0.362961	-1.940191	C	-0.991222	1.132086	6.212188
C	-0.206754	1.396399	-1.111837	C	-0.959373	3.175142	5.360963
C	-1.466760	1.282614	-0.468228	N	-1.119768	1.864898	5.070082
C	-0.165151	3.396006	0.127167	C	-0.709803	2.020348	7.440150
C	0.500264	2.619512	-0.747005	H	0.236587	1.714250	7.894999
H	-3.240041	-3.696680	-2.394021	H	-1.494999	1.862207	8.184941
H	-3.802147	-1.763559	-0.930665	C	-0.688268	3.424090	6.854001
H	0.495408	-1.852214	-3.456665	H	0.270382	3.939039	6.964766
H	-1.098292	-3.731510	-3.648909	H	-1.461448	4.086141	7.254394
H	1.096102	0.372254	-2.476550	O	-1.016759	4.107254	4.546041
Br	0.327059	4.990237	0.915728	O	-1.081697	-0.090670	6.295149
N	-2.328114	0.330345	-0.552300				

Number of imaginary frequencies = 0

Zero-point vibrational correction = 0.250868 hartree
Thermal correction to Gibbs free energy = 0.193190 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10727.4520801 hartree

TS2 of the reaction for 4g:

Atom	x	y	z	Atom	x	y	z
C	-2.514686	-2.871267	-1.846138	S	-1.859125	3.011706	0.384302
C	-2.872529	-1.724074	-1.184541	I	2.382382	3.123728	-1.467228
C	-1.976127	-0.628935	-1.131870	C	-1.529557	2.495051	2.364563
C	-0.701669	-0.729273	-1.769119	H	-0.650908	1.874509	2.243531
C	-0.364872	-1.931018	-2.445883	H	-1.394536	3.488530	2.785553
C	-1.251725	-2.975887	-2.482425	H	-2.465903	1.989984	2.563622
C	0.186462	0.370784	-1.703296	C	-1.056376	1.044310	5.440560
C	-0.212942	1.496945	-1.027082	C	-0.927235	3.269654	5.245942
C	-1.511313	1.466679	-0.446286	N	-1.141750	2.103580	4.585966
C	-0.250946	3.624512	-0.047104	C	-0.747957	1.517092	6.872230
C	0.475713	2.753938	-0.774585	H	0.179563	1.047162	7.210349
H	-3.201747	-3.709866	-1.885275	H	-1.546688	1.179263	7.538109
H	-3.832411	-1.621210	-0.690421	C	-0.657832	3.032945	6.738464
H	0.604307	-2.004086	-2.929838	H	0.322905	3.442907	6.994837
H	-0.989460	-3.892279	-3.000083	H	-1.402802	3.575066	7.327279
H	1.163140	0.315784	-2.177175	O	-0.942556	4.388232	4.729394
Br	0.206302	5.309876	0.564246	O	-1.200837	-0.134747	5.139157
N	-2.369165	0.500746	-0.468140				

Number of imaginary frequencies = 1 (-481.9558 cm^{-1})
Zero-point vibrational correction = 0.250122 hartree
Thermal correction to Gibbs free energy = 0.191338 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10727.4436350 hartree

Product of the reaction for 4g:

Atom	x	y	z	Atom	x	y	z
C	-2.346360	-2.793963	-1.644147	C	0.786467	2.666400	-0.232627
C	-2.724326	-1.612678	-1.062487	H	-3.072737	-3.589066	-1.777411
C	-1.779800	-0.566327	-0.883620	H	-3.740476	-1.439763	-0.724096
C	-0.432787	-0.763685	-1.318258	H	0.949994	-2.145222	-2.247124
C	-0.075645	-2.002966	-1.918907	H	-0.729548	-3.935363	-2.536482
C	-1.008293	-2.992607	-2.077712	H	1.529999	0.157952	-1.455935
C	0.498316	0.280875	-1.135147	Br	0.474089	5.291872	0.928201
C	0.073597	1.449015	-0.545324	N	-2.199055	0.590450	-0.300616
C	-1.300460	1.523640	-0.154489	S	-1.670439	3.082269	0.581138
C	-0.007402	3.589980	0.354571	I	2.794474	2.919696	-0.653027

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.130792 hartree

Thermal correction to Gibbs free energy = 0.089571 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10327.5974713 hartree

Reaction for 4h

Reactant1 of the reaction for 4h:

Atom	x	y	z	Atom	x	y	z
C	-1.967687	-2.543384	-1.647024	C	4.188483	6.074929	1.663789
C	-2.543615	-1.371868	-1.231267	H	3.973151	4.038655	0.990087
C	-1.731497	-0.304458	-0.769991	H	0.317265	6.228146	1.537755
C	-0.323197	-0.472987	-0.752032	C	3.526380	7.249833	2.018128
C	0.241451	-1.699677	-1.188749	H	5.272302	6.029864	1.696679
C	-0.555054	-2.728027	-1.631509	H	4.095103	8.120961	2.327334
C	0.454396	0.617177	-0.304458	N	-2.336110	0.842168	-0.344984
C	-0.156915	1.786716	0.098481	S	-2.475235	3.316537	0.562514
C	-1.596122	1.834025	0.075978	C	2.133638	7.306055	1.974492
C	1.303653	3.863567	0.819323	H	1.616657	8.219953	2.248973
C	0.625632	2.913375	0.492287	C	0.024375	-4.036576	-2.098370
H	-2.594919	-3.358607	-1.998675	H	-0.253732	-4.235741	-3.138432
H	-3.619224	-1.228730	-1.239697	H	1.114411	-4.035451	-2.029045
H	1.322842	-1.812912	-1.168776	H	-0.357476	-4.867387	-1.496115
H	1.538261	0.542988	-0.295785	C	-1.995939	3.447725	2.315165
C	2.063709	5.008005	1.221680	H	-2.561663	4.290238	2.717451
C	3.464815	4.956532	1.266878	H	-0.929081	3.644824	2.422349
C	1.401639	6.193174	1.578435	H	-2.274655	2.540925	2.853278

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.286182 hartree
Thermal correction to Gibbs free energy = 0.236788 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -1185.82127699 hartree

Entrance1 of the reaction for 4h:

Atom	x	y	z	Atom	x	y	z
C	-2.321317	-3.024600	-0.149359	C	1.527852	2.096316	-0.178123
C	-1.050287	-2.846710	0.330708	C	2.101415	3.166370	-0.239102
C	-0.396544	-1.598973	0.166147	C	2.842155	4.390012	-0.306789
C	-1.082195	-0.548916	-0.497487	C	2.308253	5.514798	-0.952939
C	-2.397357	-0.766495	-0.984169	C	4.116856	4.458789	0.275870
C	-3.020595	-1.980080	-0.820158	C	3.045670	6.690962	-1.015537
H	-2.817564	-3.982963	-0.020534	H	1.319961	5.456647	-1.397738
H	-0.515024	-3.640913	0.840499	C	4.846464	5.639653	0.206539
N	0.874736	-1.458039	0.639938	H	4.519567	3.585525	0.779358
C	-0.409840	0.685698	-0.624198	C	4.313438	6.755605	-0.437832
H	-2.908373	0.049420	-1.489383	H	2.630177	7.559543	-1.515601

C	0.864584	0.833606	-0.116137	H	5.831815	5.689926	0.657886
C	1.482507	-0.309496	0.503293	H	4.885453	7.676352	-0.488617
H	-0.905371	1.526768	-1.101657	I	-0.689240	4.111872	1.033654
S	3.126622	-0.197293	1.201323	I	-2.880567	5.370297	2.002231
C	4.112397	0.150466	-0.290711	C	-4.415205	-2.231400	-1.327407
H	3.863403	1.122370	-0.718136	H	-5.081107	-2.517884	-0.506941
H	5.154472	0.156893	0.034617	H	-4.828392	-1.343104	-1.810213
H	3.973631	-0.639553	-1.029671	H	-4.422884	-3.051745	-2.052522

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.287083 hartree
Thermal correction to Gibbs free energy = 0.225367 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8025010 hartree

TS1 of the reaction for 4h:

Atom	x	y	z	Atom	x	y	z
C	0.000000	0.000000	0.000000	C	1.155005	0.000559	-2.250558
C	0.000000	0.000000	1.370258	H	3.349132	0.000247	-0.613917
C	1.227350	0.000000	2.078962	H	4.602597	-0.004367	1.558267
C	2.444323	-0.000087	1.349278	H	3.097954	-2.258471	5.696425
C	2.408835	0.000057	-0.068465	H	1.309264	-2.209557	5.784570
C	1.213106	0.000182	-0.746810	H	2.287566	-1.933397	7.252193
C	3.652270	-0.001755	2.084085	C	5.840279	-1.329525	7.403547
N	1.195511	0.002581	3.443853	C	5.650625	1.097418	7.628657
C	3.616271	-0.000788	3.457005	C	6.370615	-1.399642	8.683167
C	2.324650	0.000156	4.093752	C	6.536940	-0.232760	9.431475
C	4.791328	-0.011685	4.310194	C	6.178339	1.011847	8.907279
C	4.942850	-0.008641	5.565147	H	5.709206	-2.223147	6.802110
C	5.481754	-0.076324	6.869585	H	5.362778	2.052563	7.202845
I	6.913498	-0.062512	3.359882	H	6.655804	-2.359305	9.099496
I	9.468070	-0.138068	1.808450	H	6.950814	-0.292827	10.432800
S	2.257596	0.012843	5.884206	H	6.313423	1.910448	9.498769
C	2.236292	-1.785677	6.172116	H	0.620192	0.882561	-2.617425
H	-0.943312	0.000304	-0.539610	H	2.156214	-0.000100	-2.686662
H	-0.921519	0.000634	1.942660	H	0.618707	-0.880331	-2.617924

Number of imaginary frequencies = 1 (-178.8542 cm^{-1})
Zero-point vibrational correction = 0.286919 hartree
Thermal correction to Gibbs free energy = 0.229023 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.7898556 hartree

IM of the reaction for 4h:

Atom	x	y	z	Atom	x	y	z
C	-2.331873	-2.647898	-1.953753	H	1.643861	4.226101	2.491498
C	-2.724706	-1.378350	-1.621839	H	-0.755407	6.055800	-0.579278

C	-1.760439	-0.426905	-1.210096	C	0.966666	7.513080	1.957661
C	-0.386211	-0.806868	-1.144603	H	2.140694	6.460371	3.425653
C	-0.021622	-2.131111	-1.499454	H	1.180309	8.492695	2.372254
C	-0.965515	-3.047083	-1.898545	N	-2.178677	0.837568	-0.894398
C	0.572003	0.148698	-0.724891	S	-1.607636	3.354045	-0.073907
C	0.142562	1.409864	-0.389211	I	2.968431	2.480317	0.306838
C	-1.249041	1.645915	-0.514516	C	0.145179	7.394519	0.838186
C	0.125581	3.660687	0.342434	H	-0.279078	8.278991	0.375237
C	0.884332	2.573521	0.091864	C	-0.593022	-4.454367	-2.277124
H	-3.074064	-3.375802	-2.269704	H	-0.893194	-4.668759	-3.307777
H	-3.763772	-1.070462	-1.665060	H	0.482980	-4.617691	-2.190313
H	1.027231	-2.410987	-1.449081	H	-1.105282	-5.175767	-1.632519
H	1.623741	-0.118465	-0.667288	C	-2.375075	3.165769	1.564196
C	0.423933	4.991536	0.887678	H	-3.370177	2.752238	1.396359
C	1.236845	5.115088	2.022044	H	-1.758080	2.505194	2.172646
C	-0.129452	6.140026	0.305056	H	-2.441723	4.165492	1.995623
C	1.509334	6.372838	2.547984	I	6.389096	2.199227	0.644809

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.289853 hartree
Thermal correction to Gibbs free energy = 0.233732 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8254208 hartree

Reactant2 of the reaction for 4h:

Atom	x	y	z	Atom	x	y	z
C	-2.335855	-2.654932	-1.943547	H	1.578652	4.208836	2.535526
C	-2.728244	-1.386804	-1.605690	H	-0.690517	6.061159	-0.622199
C	-1.761602	-0.435165	-1.201467	C	0.979904	7.503663	1.958326
C	-0.385335	-0.813011	-1.150294	H	2.085065	6.441235	3.472014
C	-0.021649	-2.135661	-1.510774	H	1.196321	8.481835	2.374684
C	-0.968391	-3.052306	-1.902027	N	-2.178714	0.827627	-0.878943
C	0.574890	0.143795	-0.739223	S	-1.608572	3.346033	-0.063068
C	0.143593	1.402250	-0.397728	I	2.934020	2.520684	0.259101
C	-1.248924	1.637563	-0.506347	C	0.192408	7.393635	0.813640
C	0.120215	3.661220	0.341265	H	-0.201553	8.282813	0.333642
C	0.874078	2.574367	0.075262	C	-0.598395	-4.458474	-2.285894
H	-3.079668	-3.383481	-2.253779	H	-0.908638	-4.671302	-3.313804
H	-3.768094	-1.080702	-1.638455	H	0.478361	-4.621518	-2.209319
H	1.027892	-2.414504	-1.471357	H	-1.104811	-5.180477	-1.637473
H	1.627549	-0.122287	-0.693142	C	-2.368823	3.168298	1.579909
C	0.427519	4.988871	0.886670	H	-3.364545	2.755218	1.413963
C	1.206320	5.102549	2.045734	H	-1.752299	2.510181	2.191283
C	-0.088968	6.141354	0.279178	H	-2.434366	4.171596	2.003136
C	1.483442	6.358405	2.573336				

Number of imaginary frequencies = 0

Zero-point vibrational correction = 0.288973 hartree
Thermal correction to Gibbs free energy = 0.240691 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8076.15909099 hartree

Entrance2 of the reaction for 4h:

Atom	x	y	z	Atom	x	y	z
C	-2.329203	-2.653632	-1.959938	H	1.555621	4.205597	2.540958
C	-2.721472	-1.385276	-1.623553	H	-0.672137	6.058260	-0.643848
C	-1.755657	-0.433229	-1.216787	C	0.988494	7.502409	1.942473
C	-0.380219	-0.811794	-1.161875	H	2.069464	6.438993	3.472830
C	-0.016220	-2.134986	-1.521467	H	1.206651	8.480856	2.357407
C	-0.961909	-3.051394	-1.914676	N	-2.174427	0.828457	-0.894122
C	0.578613	0.144657	-0.747369	S	-1.611181	3.340640	-0.059679
C	0.145934	1.402388	-0.405503	I	2.934597	2.524170	0.257000
C	-1.246813	1.640154	-0.516916	C	0.210483	7.392745	0.791300
C	0.117014	3.659108	0.333875	H	-0.174438	8.282450	0.304879
C	0.873929	2.574074	0.069927	C	-0.591430	-4.458543	-2.295429
H	-3.072803	-3.382413	-2.270344	H	-0.901451	-4.674607	-3.322799
H	-3.761258	-1.078908	-1.656690	H	0.485489	-4.620981	-2.218363
H	1.033080	-2.414471	-1.477920	H	-1.097049	-5.179282	-1.644927
H	1.631077	-0.121605	-0.697625	C	-2.364009	3.140189	1.603061
C	0.428012	4.986951	0.877442	H	-3.355119	2.716344	1.444241
C	1.197273	5.100301	2.042558	H	-1.735854	2.484694	2.203446
C	-0.075301	6.139930	0.260463	H	-2.439233	4.136311	2.038161
C	1.477871	6.356548	2.567482	I	-3.849639	2.795206	4.687252

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.289709 hartree
Thermal correction to Gibbs free energy = 0.232932 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8261724 hartree

TS2 of the reaction for 4h:

Atom	x	y	z	Atom	x	y	z
C	-2.337222	-2.610331	-2.024171	H	1.461351	4.238323	2.571352
C	-2.720532	-1.333217	-1.715719	H	-0.612820	6.062305	-0.726801
C	-1.759440	-0.391167	-1.267468	C	0.974898	7.532371	1.891774
C	-0.396155	-0.796640	-1.144104	H	1.977180	6.479595	3.481756
C	-0.040281	-2.131225	-1.476649	H	1.195458	8.514888	2.295944
C	-0.980388	-3.033294	-1.909315	N	-2.174525	0.874732	-0.971372
C	0.556402	0.144070	-0.689532	S	-1.612849	3.368671	-0.107015
C	0.131303	1.414409	-0.380221	I	2.906055	2.498152	0.399721
C	-1.252835	1.688238	-0.559285	C	0.239626	7.412725	0.713896
C	0.090765	3.671535	0.317551	H	-0.110250	8.299251	0.195826
C	0.854577	2.573777	0.114357	C	-0.617878	-4.450136	-2.262536
H	-3.078398	-3.327833	-2.365757	H	-0.876546	-4.667799	-3.303834

H	-3.751889	-1.008476	-1.801989	H	0.450381	-4.632341	-2.127951
H	1.000714	-2.428854	-1.379713	H	-1.169980	-5.158198	-1.636175
H	1.600079	-0.140869	-0.584340	C	-2.411206	3.021763	1.885467
C	0.410619	5.003960	0.851721	H	-3.352300	2.594537	1.567240
C	1.136642	5.128814	2.043005	H	-1.623817	2.359268	2.219167
C	-0.048046	6.154187	0.196768	H	-2.394985	4.052875	2.210928
C	1.418760	6.390095	2.556025	I	-3.435685	2.562158	4.466372

Number of imaginary frequencies = 1 (-492.4447 cm^{-1})
Zero-point vibrational correction = 0.288394 hartree
Thermal correction to Gibbs free energy = 0.232284 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8178808 hartree

Product of the reaction for 4h:

Atom	x	y	z	Atom	x	y	z
C	-2.331795	-2.625559	-2.011576	C	-0.099762	6.113794	0.248612
C	-2.726340	-1.364688	-1.659480	C	1.477290	6.396449	2.527348
C	-1.773049	-0.414145	-1.200193	H	1.510460	4.245632	2.588291
C	-0.402174	-0.804949	-1.115992	H	-0.708672	6.002144	-0.643969
C	-0.033891	-2.127497	-1.492799	C	1.009196	7.526966	1.859635
C	-0.965400	-3.031771	-1.933176	H	2.081584	6.503065	3.422322
C	0.541223	0.138521	-0.659460	H	1.255326	8.517255	2.229006
C	0.103976	1.396907	-0.309307	N	-2.205982	0.829117	-0.860259
C	-1.293546	1.665204	-0.442004	S	-1.666669	3.311705	0.045285
C	0.030170	3.631556	0.410003	I	2.887762	2.513555	0.381653
C	0.819836	2.552469	0.177501	C	0.218829	7.383013	0.721124
H	-3.068707	-3.344189	-2.360884	H	-0.149919	8.259318	0.198176
H	-3.764299	-1.053973	-1.718301	C	-0.588293	-4.432845	-2.333842
H	1.013816	-2.410769	-1.423593	H	-0.856855	-4.624870	-3.377904
H	1.592302	-0.130005	-0.585825	H	0.484562	-4.603219	-2.219292
C	0.379435	4.974384	0.906593	H	-1.120116	-5.169203	-1.722316
C	1.163646	5.125737	2.056660				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.250481 hartree
Thermal correction to Gibbs free energy = 0.203359 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8036.47942331 hartree

Reaction for 4i

Reactant1 of the reaction for 4i:

Atom	x	y	z	Atom	x	y	z
C	-1.531143	-2.818462	-1.234167	H	0.375874	6.148097	1.763776

C	-1.725029	-1.960554	-0.177325	C	2.491375	7.543775	-1.169224
C	-1.159352	-0.660872	-0.178054	H	2.259871	5.593398	-2.057473
C	-0.383269	-0.238783	-1.288135	C	2.194801	8.357035	-0.076104
C	-0.189184	-1.133771	-2.373272	H	1.202144	8.487494	1.831526
C	-0.747883	-2.383327	-2.341972	H	3.082189	7.932421	-1.992463
C	0.145415	1.068376	-1.256832	H	2.554873	9.380494	-0.047723
C	-0.093203	1.887245	-0.171581	N	-1.370404	0.140757	0.906632
C	-0.861037	1.344655	0.918706	S	-1.240983	2.338303	2.359477
C	0.793530	4.372971	-0.176423	C	-2.123403	-4.202127	-1.248677
C	0.384115	3.231973	-0.162738	H	-2.789003	-4.330018	-2.108609
H	-2.313487	-2.255015	0.686781	H	-1.337194	-4.959592	-1.332466
H	0.404892	-0.809979	-3.223211	H	-2.695082	-4.399083	-0.339297
H	0.724957	1.439764	-2.097497	H	-0.597367	-3.065322	-3.174699
C	1.268101	5.723302	-0.149922	C	0.427409	2.658902	3.016800
C	0.971194	6.546057	0.947743	H	0.279737	3.194312	3.956680
C	2.032591	6.232373	-1.210367	H	1.012079	3.278053	2.336153
C	1.434817	7.855755	0.980301	H	0.942407	1.718950	3.218733

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.286137 hartree
Thermal correction to Gibbs free energy = 0.236765 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -1185.82152569 hartree

Entrance1 of the reaction for 4i:

Atom	x	y	z	Atom	x	y	z
C	-2.334494	-3.047063	-0.141329	C	2.104292	3.166190	-0.245233
C	-1.059293	-2.843133	0.331498	C	2.847054	4.388591	-0.314066
C	-0.408581	-1.595652	0.161743	C	2.315804	5.513089	-0.962943
C	-1.085941	-0.541154	-0.504073	C	4.121214	4.456463	0.269901
C	-2.401655	-0.763794	-0.989132	C	3.055390	6.687799	-1.027240
C	-3.002401	-1.981088	-0.810601	H	1.327861	5.455845	-1.408652
H	-0.516157	-3.630801	0.845253	C	4.852981	5.635910	0.198882
N	0.863740	-1.456123	0.636292	H	4.521894	3.583632	0.775762
C	-0.411763	0.690510	-0.632317	C	4.322686	6.751465	-0.448394
H	-2.919424	0.044439	-1.497403	H	5.837929	5.685366	0.651210
C	0.863028	0.835912	-0.123033	H	4.896411	7.671070	-0.500540
C	1.474582	-0.309333	0.497886	H	-4.009873	-2.147878	-1.182019
H	-0.904841	1.532037	-1.111598	I	-0.678438	4.114162	1.029803
S	3.118816	-0.203577	1.197399	I	-2.867006	5.376235	2.000999
C	4.107193	0.150490	-0.291441	C	-3.039868	-4.365382	0.029559
H	3.864916	1.127266	-0.711383	H	-2.414091	-5.085070	0.561484
H	5.149014	0.147302	0.034735	H	-3.970909	-4.236425	0.591118
H	3.963965	-0.632789	-1.036693	H	-3.305086	-4.791698	-0.943474
C	1.529359	2.096739	-0.184514	H	2.641901	7.556060	-1.529529

Number of imaginary frequencies = 0

Zero-point vibrational correction = 0.287062 hartree
Thermal correction to Gibbs free energy = 0.225457 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8028182 hartree

TS1 of the reaction for 4i:

Atom	x	y	z	Atom	x	y	z
C	0.000000	0.000000	0.000000	H	1.240529	0.000576	-1.776880
C	0.000000	0.000000	1.375416	H	3.382073	0.001123	-0.550351
C	1.215086	0.000000	2.102863	H	4.602964	-0.003659	1.656544
C	2.450663	0.000373	1.404373	H	3.002586	-2.263223	5.754072
C	2.437390	0.000645	-0.014714	H	1.212434	-2.209302	5.801684
C	1.246118	0.000369	-0.690337	H	2.157964	-1.940882	7.292145
C	3.641971	-0.001225	2.162684	C	5.709888	-1.333364	7.531112
N	1.155671	0.002084	3.468155	C	5.523862	1.094490	7.748913
C	3.576960	-0.000789	3.535114	C	6.212459	-1.403521	8.821870
C	2.271211	-0.000368	4.141034	C	6.366945	-0.236136	9.571972
C	4.732526	-0.012346	4.413950	C	6.024002	1.008971	9.038587
C	4.856712	-0.011608	5.672073	H	5.588396	-2.227403	6.928296
C	5.367148	-0.079712	6.987867	H	5.248616	2.050030	7.315713
I	6.873796	-0.057414	3.509732	H	6.485255	-2.363564	9.245565
I	9.463656	-0.123650	2.014743	H	6.759195	-0.296267	10.581964
S	2.164824	0.009746	5.930309	H	6.149692	1.907958	9.631563
C	2.131659	-1.789569	6.211684	H	-2.152841	-0.000545	-0.134013
C	-1.280246	0.000294	-0.790499	H	-1.335227	0.882266	-1.436839
H	-0.927899	0.000468	1.939327	H	-1.334681	-0.880415	-1.438617

Number of imaginary frequencies = 1 (-177.6120 cm^{-1})
Zero-point vibrational correction = 0.286932 hartree
Thermal correction to Gibbs free energy = 0.229018 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.7901150 hartree

IM of the reaction for 4i:

Atom	x	y	z	Atom	x	y	z
C	-1.922657	-3.076092	-1.131042	C	1.847844	6.737611	1.385315
C	-2.109207	-2.040545	-0.245433	H	2.337039	4.808801	0.565474
C	-1.476082	-0.791873	-0.447114	C	0.829927	7.581048	1.827536
C	-0.630340	-0.596959	-1.580395	H	-1.292168	7.810176	2.122180
C	-0.452622	-1.677888	-2.483976	H	2.882331	7.060780	1.429765
C	-1.079455	-2.874300	-2.261466	H	1.070661	8.566697	2.211884
C	0.002663	0.654676	-1.765966	N	-1.704429	0.209170	0.460592
C	-0.214883	1.646779	-0.839685	S	-1.276782	2.745283	1.306767
C	-1.086875	1.316078	0.226500	I	1.581520	3.745628	-2.252163
C	-0.104858	3.706633	0.320491	C	-2.586341	-4.411347	-0.936041
C	0.313442	3.005916	-0.754134	H	-3.220530	-4.654822	-1.794446
H	-2.745241	-2.152027	0.627221	H	-1.837039	-5.204906	-0.850694

H	0.187373	-1.536930	-3.349539	H	-3.204238	-4.421165	-0.036007
H	0.650569	0.820713	-2.622448	H	-0.937091	-3.695656	-2.958101
C	0.211586	5.047437	0.830271	C	-0.275278	2.256549	2.743877
C	-0.807373	5.894448	1.286954	H	-0.836557	1.479029	3.263433
C	1.544810	5.473011	0.893571	H	0.692715	1.895208	2.397863
C	-0.496721	7.156784	1.780263	H	-0.174146	3.142730	3.371786
H	-1.845135	5.576435	1.233751	I	3.653660	4.882701	-4.761251

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.289677 hartree
Thermal correction to Gibbs free energy = 0.233367 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8256175 hartree

Reactant2 of the reaction for 4i:

Atom	x	y	z	Atom	x	y	z
C	-1.920574	-3.080434	-1.129217	C	1.853550	6.717384	1.416838
C	-2.098276	-2.048241	-0.237436	H	2.338310	4.767807	0.643076
C	-1.471789	-0.797818	-0.444406	C	0.834205	7.582514	1.811700
C	-0.641557	-0.596842	-1.589059	H	-1.292173	7.850776	2.032897
C	-0.472990	-1.674022	-2.498578	H	2.890874	7.024461	1.495037
C	-1.093705	-2.872562	-2.270683	H	1.077887	8.569120	2.191516
C	-0.015589	0.657021	-1.779392	N	-1.691030	0.200249	0.468664
C	-0.225468	1.643663	-0.846165	S	-1.265141	2.735598	1.318696
C	-1.081113	1.309400	0.231248	I	1.515502	3.768403	-2.233706
C	-0.113092	3.706984	0.328379	C	-2.577105	-4.418090	-0.929671
C	0.288963	3.005908	-0.752076	H	-3.218451	-4.662023	-1.782499
H	-2.721903	-2.164178	0.643402	H	-1.823480	-5.208446	-0.853635
H	0.154309	-1.529167	-3.372715	H	-3.185761	-4.431884	-0.023598
H	0.619582	0.826817	-2.644617	H	-0.959289	-3.691439	-2.971688
C	0.208510	5.048689	0.830165	C	-0.245370	2.252034	2.745518
C	-0.812989	5.915416	1.241257	H	-0.800281	1.471179	3.267079
C	1.546459	5.451474	0.931433	H	0.720462	1.894555	2.390068
C	-0.497409	7.179710	1.725946	H	-0.144759	3.137671	3.374292
H	-1.852673	5.610297	1.160492				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.289657 hartree
Thermal correction to Gibbs free energy = 0.240085 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8076.15935598 hartree

Entrance2 of the reaction for 4i:

Atom	x	y	z	Atom	x	y	z
C	-1.926608	-3.074999	-1.133510	C	1.843637	6.719986	1.410505
C	-2.108788	-2.039767	-0.246724	H	2.328829	4.767798	0.643597
C	-1.479861	-0.789928	-0.453294	C	0.824024	7.587371	1.799328

C	-0.643092	-0.593686	-1.593486	H	-1.302843	7.858454	2.012388
C	-0.470331	-1.674114	-2.498660	H	2.881286	7.023928	1.496449
C	-1.093055	-2.871515	-2.270975	H	1.067728	8.573191	2.181291
C	-0.014805	0.659021	-1.783310	N	-1.702274	0.209147	0.456986
C	-0.228186	1.647453	-0.853076	S	-1.267519	2.739253	1.312499
C	-1.089250	1.318324	0.222736	I	1.518268	3.769873	-2.238228
C	-0.123254	3.710888	0.317913	C	-2.583652	-4.412353	-0.931688
C	0.285422	3.009230	-0.759540	H	-3.220366	-4.661360	-1.786644
H	-2.735584	-2.152755	0.632252	H	-1.830036	-5.201843	-0.846882
H	0.163317	-1.532676	-3.368854	H	-3.197025	-4.422117	-0.028663
H	0.625918	0.825935	-2.645030	H	-0.954017	-3.693124	-2.967978
C	0.198855	5.053696	0.816828	C	-0.225704	2.246815	2.742151
C	-0.822882	5.922181	1.223058	H	-0.761543	1.449251	3.255785
C	1.536769	5.454328	0.924222	H	0.742584	1.909219	2.377829
C	-0.507778	7.186624	1.707671	H	-0.133739	3.122781	3.383872
H	-1.862280	5.616501	1.140926	I	1.662901	1.155698	5.403567

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.289546 hartree
Thermal correction to Gibbs free energy = 0.232534 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8263929 hartree

TS2 of the reaction for 4i:

Atom	x	y	z	Atom	x	y	z
C	-1.966469	-3.056700	-1.140281	C	1.788561	6.727909	1.448740
C	-2.167986	-2.012377	-0.270643	H	2.296569	4.767706	0.719130
C	-1.508101	-0.771564	-0.453847	C	0.758257	7.600947	1.794173
C	-0.618738	-0.602030	-1.558154	H	-1.374186	7.874410	1.933929
C	-0.424408	-1.694613	-2.446773	H	2.823409	7.032032	1.564679
C	-1.077457	-2.878538	-2.240962	H	0.990242	8.591300	2.171958
C	0.037024	0.636730	-1.728651	N	-1.752462	0.231656	0.440604
C	-0.204351	1.639199	-0.818532	S	-1.304521	2.749544	1.299640
C	-1.119444	1.343278	0.228491	I	1.613560	3.731304	-2.158195
C	-0.149682	3.701578	0.332801	C	-2.658287	-4.380094	-0.960092
C	0.316393	2.991896	-0.720376	H	-3.261188	-4.623736	-1.840869
H	-2.836720	-2.107849	0.579304	H	-1.925837	-5.184308	-0.835917
H	0.250907	-1.570328	-3.288088	H	-3.312118	-4.371312	-0.085675
H	0.719516	0.785867	-2.561306	H	-0.921995	-3.708163	-2.925063
C	0.162602	5.053524	0.819924	C	0.020242	2.128105	2.907595
C	-0.869232	5.928254	1.183777	H	-0.597392	1.317066	3.269147
C	1.495810	5.456977	0.966490	H	0.870005	1.896729	2.279656
C	-0.569749	7.198846	1.663338	H	0.013955	3.063888	3.449967
H	-1.904906	5.619290	1.072812	I	1.763240	1.310288	4.962576

Number of imaginary frequencies = 1 (-489.2584 cm^{-1})
Zero-point vibrational correction = 0.288243 hartree

Thermal correction to Gibbs free energy = 0.231938 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8181091 hartree

Product of the reaction for 4i:

Atom	x	y	z	Atom	x	y	z
C	5.705699	-0.529941	0.030444	C	-4.814965	-2.267183	-0.810921
C	4.629788	-1.380609	0.057245	H	-2.806021	-2.576963	-1.516529
C	3.296634	-0.886906	0.047584	C	-5.073520	-0.650464	0.960546
C	3.076546	0.523921	0.009110	H	-3.264626	0.283469	1.656714
C	4.207045	1.389459	-0.017511	C	-5.633349	-1.571605	0.076687
C	5.474272	0.878508	-0.006962	H	-5.244637	-2.986642	-1.500235
C	1.752458	1.005477	-0.001534	H	-5.704695	-0.116184	1.663161
C	0.717501	0.096350	0.029326	H	-6.703710	-1.750357	0.083652
C	1.066776	-1.288821	0.063943	N	2.275378	-1.785070	0.073745
C	-1.419321	-0.878533	0.053200	S	-0.371044	-2.297962	0.096839
C	-0.714378	0.280811	0.020518	I	-1.540974	2.181193	-0.132411
H	4.765391	-2.457834	0.086016	C	7.120892	-1.041840	0.038852
H	4.040652	2.462640	-0.046370	H	7.658890	-0.708861	-0.854917
H	1.558883	2.075101	-0.032686	H	7.667221	-0.657886	0.906713
C	-2.875412	-1.106172	0.057319	H	7.148779	-2.133181	0.070141
C	-3.442258	-2.040688	-0.818289	H	6.330083	1.547880	-0.027502
C	-3.701992	-0.418682	0.954434				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.250512 hartree
Thermal correction to Gibbs free energy = 0.203437 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8036.47984488 hartree

Reaction for 4j

Reactant1 of the reaction for 4j:

Atom	x	y	z	Atom	x	y	z
C	-2.350041	-2.942993	0.064139	H	5.146037	0.056831	-0.939809
C	-0.993293	-2.864228	0.257383	H	3.706073	-0.470578	-1.838823
C	-0.333342	-1.613908	0.158346	C	1.664449	2.062277	0.003133
C	-1.089862	-0.449823	-0.138868	C	2.243229	3.127396	0.006594
C	-2.490816	-0.559321	-0.335032	C	2.969084	4.361251	0.011637
C	-3.105867	-1.781582	-0.235234	C	2.318716	5.574951	-0.256065
H	-2.853760	-3.901293	0.139652	C	4.346082	4.357598	0.283642
H	-0.394348	-3.739810	0.485224	C	3.038274	6.764106	-0.251171
N	1.019732	-1.576031	0.338891	H	1.254018	5.573715	-0.465567
C	-0.394981	0.778089	-0.208088	C	5.057239	5.551470	0.285570
H	-3.061524	0.336737	-0.561552	H	4.842971	3.415582	0.494398
C	0.966979	0.817378	0.004208	C	4.406301	6.755511	0.018601

C	1.642135	-0.430371	0.258834	H	2.530314	7.700445	-0.458525
H	-0.938303	1.697467	-0.407935	H	6.121692	5.542974	0.496797
S	3.404932	-0.476736	0.569153	H	4.964490	7.686270	0.021589
C	4.060442	0.146350	-1.012175	H	-4.177336	-1.865188	-0.384713
H	3.793667	1.191180	-1.171361				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.258306 hartree
Thermal correction to Gibbs free energy = 0.209864 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -1146.51350270 hartree

Entrance1 of the reaction for 4j:

Atom	x	y	z	Atom	x	y	z
C	-2.326083	-3.031126	-0.146796	H	3.966531	-0.630500	-1.038170
C	-1.052616	-2.847594	0.332372	C	1.526376	2.096751	-0.181626
C	-0.403997	-1.599051	0.163444	C	2.101172	3.166193	-0.240828
C	-1.086333	-0.545973	-0.501427	C	2.842838	4.389345	-0.306385
C	-2.401329	-0.762344	-0.987978	C	2.310568	5.514902	-0.952525
C	-3.006686	-1.981072	-0.813140	C	4.116793	4.456669	0.278095
H	-2.821090	-3.987988	-0.017050	C	3.049020	6.690496	-1.013437
H	-0.512475	-3.637361	0.843666	H	1.322857	5.457757	-1.398731
N	0.869070	-1.457474	0.636759	C	4.847381	5.637001	0.210468
C	-0.412207	0.688358	-0.628747	H	4.518157	3.582819	0.781646
H	-2.914916	0.049917	-1.493878	C	4.316059	6.753728	-0.433985
C	0.861634	0.834879	-0.121209	H	2.634899	7.559707	-1.513526
C	1.477665	-0.310554	0.498677	H	5.832152	5.686271	0.663172
H	-0.907428	1.529512	-1.106339	H	4.888904	7.674026	-0.483464
S	3.122125	-0.201216	1.196223	H	-4.012589	-2.146971	-1.184097
C	4.107684	0.154347	-0.294206	I	-0.691344	4.114027	1.029208
H	3.861684	1.129740	-0.715134	I	-2.882833	5.374075	1.994697
H	5.149735	0.155233	0.031199				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.259316 hartree
Thermal correction to Gibbs free energy = 0.199803 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14927.4945917 hartree

TS1 of the reaction for 4j:

Atom	x	y	z	Atom	x	y	z
C	-1.799346	-3.204163	0.018578	H	3.297242	-0.073508	-2.010700
C	-0.505283	-2.747644	0.063353	C	0.691144	2.747266	0.083543
C	-0.247044	-1.355154	0.070385	C	1.827860	3.299015	0.126707
C	-1.334236	-0.442133	0.030572	C	2.886242	4.234856	0.100724
C	-2.660780	-0.941166	-0.014873	C	3.325691	4.746720	-1.135808
C	-2.885715	-2.294907	-0.020596	C	3.500024	4.642633	1.300499

H	-1.997617	-4.270882	0.013540	C	4.364887	5.664843	-1.163706
H	0.341949	-3.424273	0.094769	H	2.837119	4.426315	-2.050151
N	1.052734	-0.934384	0.118583	C	4.539836	5.557822	1.257101
C	-1.037102	0.940835	0.036529	H	3.152091	4.232429	2.242408
H	-3.486543	-0.236685	-0.044614	C	4.969722	6.066545	0.028749
C	0.269821	1.357538	0.082639	H	4.704993	6.069365	-2.110458
C	1.294250	0.344810	0.122672	H	5.017814	5.878614	2.175921
H	-1.845891	1.665116	0.004048	H	5.783664	6.783726	0.001439
S	3.005878	0.870945	0.196044	H	-3.900443	-2.676894	-0.055103
C	3.349678	0.931904	-1.591643	I	-0.901071	4.438266	-0.028178
H	2.639357	1.591127	-2.094739	I	-3.201103	6.342054	-0.178522
H	4.360206	1.327871	-1.705215				

Number of imaginary frequencies = 1 (-180.7562 cm^{-1})
Zero-point vibrational correction = 0.259196 hartree
Thermal correction to Gibbs free energy = 0.203626 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14927.4817338 hartree

IM of the reaction for 4j:

Atom	x	y	z	Atom	x	y	z
C	-1.809912	-3.122721	0.067312	H	3.821285	-0.192884	-1.082506
C	-0.539190	-2.630933	0.233113	C	0.696621	2.841115	-0.119139
C	-0.306347	-1.238471	0.143691	C	2.030637	2.912263	0.069977
C	-1.394787	-0.351956	-0.119263	C	2.994462	4.019972	0.026311
C	-2.695206	-0.894957	-0.283251	C	2.948604	4.943897	-1.025820
C	-2.895188	-2.249125	-0.192260	C	3.984774	4.141319	1.010898
H	-1.989936	-4.190218	0.135909	C	3.867547	5.985875	-1.076047
H	0.306367	-3.279499	0.434410	H	2.200296	4.837042	-1.803640
N	0.972355	-0.777967	0.322204	C	4.902148	5.184575	0.952839
C	-1.144649	1.040063	-0.212097	H	4.022935	3.435023	1.835869
H	-3.522052	-0.220177	-0.481947	C	4.843457	6.109097	-0.088339
C	0.142713	1.490638	-0.052385	H	3.824973	6.697896	-1.893218
C	1.118604	0.497082	0.214103	H	5.658973	5.277430	1.724324
H	-1.959533	1.730861	-0.411106	H	5.559647	6.922911	-0.131962
S	2.726884	1.280395	0.423473	H	-3.891144	-2.659417	-0.319157
C	3.547843	0.861029	-1.144631	I	-0.565271	4.484099	-0.447453
H	2.861907	1.054463	-1.968879	I	-2.732656	7.104165	-0.997116
H	4.438756	1.487497	-1.207261				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.262071 hartree
Thermal correction to Gibbs free energy = 0.208414 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14927.5172260 hartree

Reactant2 of the reaction for 4j:

Atom	x	y	z	Atom	x	y	z
C	-1.801422	-3.139238	0.064756	H	4.431556	1.505218	-1.234571
C	-0.530011	-2.646305	0.222716	H	3.840941	-0.184640	-1.107556
C	-0.301060	-1.253478	0.136411	C	0.704213	2.819784	-0.108053
C	-1.393682	-0.367747	-0.115143	C	2.039545	2.898886	0.068553
C	-2.694213	-0.911969	-0.271467	C	2.993931	4.013562	0.027989
C	-2.890331	-2.266928	-0.183601	C	2.966743	4.915799	-1.043414
H	-1.979155	-4.207171	0.131019	C	3.956458	4.159068	1.036355
H	0.318008	-3.294132	0.415268	C	3.878037	5.964402	-1.089303
N	0.977721	-0.790685	0.306870	H	2.243718	4.784370	-1.841581
C	-1.147290	1.024821	-0.203245	C	4.864389	5.210607	0.982971
H	-3.523920	-0.238331	-0.461651	H	3.980742	3.465536	1.872331
C	0.140783	1.474473	-0.050945	C	4.824673	6.114757	-0.077014
C	1.122243	0.483797	0.202710	H	3.854380	6.659013	-1.922014
H	-1.966519	1.713479	-0.392023	H	5.600513	5.324656	1.771217
S	2.732468	1.267796	0.405565	H	5.535338	6.933477	-0.117314
C	3.550656	0.864789	-1.169521	H	-3.886213	-2.679085	-0.304228
H	2.857218	1.046656	-1.989923	I	-0.524762	4.458037	-0.398073

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.262078 hartree
Thermal correction to Gibbs free energy = 0.215128 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8036.85066916 hartree

Entrance2 of the reaction for 4j:

Atom	x	y	z	Atom	x	y	z
C	-3.583690	-5.030399	1.406754	H	2.246505	-2.372674	0.723681
C	-2.339695	-4.533985	1.706222	C	-0.862999	0.803365	0.801494
C	-2.047865	-3.171751	1.460478	C	0.426798	0.887682	1.187430
C	-3.050221	-2.320658	0.902065	C	1.413409	1.974026	1.140151
C	-4.325730	-2.867295	0.606973	C	1.607114	2.686488	-0.050182
C	-4.583427	-4.191747	0.853777	C	2.188394	2.276829	2.267510
H	-3.808286	-6.075074	1.593346	C	2.549693	3.706956	-0.100588
H	-1.558693	-5.156002	2.129323	H	1.032600	2.426708	-0.933251
N	-0.798570	-2.706012	1.775703	C	3.128002	3.299934	2.209352
C	-2.740661	-0.959989	0.656480	H	2.042503	1.726537	3.192933
H	-5.086605	-2.219958	0.182211	C	3.307493	4.016867	1.027629
C	-1.479633	-0.509497	0.957823	H	2.699904	4.252461	-1.025940
C	-0.588841	-1.462491	1.514547	H	3.718887	3.536970	3.087424
H	-3.490119	-0.296894	0.232506	H	4.044005	4.812308	0.983467
S	0.996413	-0.683687	1.858799	H	-5.559326	-4.605813	0.624515
C	2.036202	-1.329674	0.488536	I	-1.960464	2.401112	0.076351
H	1.494567	-1.230796	-0.449806	I	3.811835	-2.448258	-2.232544
H	2.953553	-0.741273	0.485619				

Number of imaginary frequencies = 0

Zero-point vibrational correction = 0.261826 hartree
Thermal correction to Gibbs free energy = 0.206778 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14927.5179792 hartree

TS2 of the reaction for 4j:

Atom	x	y	z	Atom	x	y	z
C	-1.785857	-3.130418	0.139086	H	3.708318	-0.254233	-1.297648
C	-0.523851	-2.629110	0.330685	C	0.724132	2.815235	-0.131101
C	-0.286615	-1.237363	0.206281	C	2.053657	2.882964	0.109149
C	-1.370668	-0.365594	-0.119578	C	2.999064	4.009035	0.076134
C	-2.664799	-0.919279	-0.310284	C	3.015756	4.880676	-1.020145
C	-2.865863	-2.269085	-0.183975	C	3.917142	4.190183	1.118562
H	-1.964902	-4.196198	0.234029	C	3.924315	5.932583	-1.058087
H	0.316554	-3.268660	0.577715	H	2.329968	4.720789	-1.845745
N	0.983391	-0.774551	0.406907	C	4.821495	5.245814	1.075682
C	-1.120208	1.020571	-0.246924	H	3.908933	3.516030	1.970470
H	-3.485547	-0.253017	-0.558429	C	4.824698	6.119141	-0.010463
C	0.161376	1.477637	-0.055592	H	3.935309	6.600779	-1.912611
C	1.145397	0.503987	0.274205	H	5.522709	5.385968	1.891375
H	-1.929567	1.701749	-0.496679	H	5.533239	6.940208	-0.044016
S	2.733998	1.276393	0.473983	H	-3.855828	-2.687017	-0.332000
C	3.574253	0.804725	-1.473026	I	-0.489546	4.451022	-0.512661
H	2.722868	1.133042	-2.053563	I	4.621192	0.207856	-4.020873
H	4.437424	1.452824	-1.404023				

Number of imaginary frequencies = 1 (-490.6951 cm^{-1})
Zero-point vibrational correction = 0.260666 hartree
Thermal correction to Gibbs free energy = 0.207056 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14927.5099441 hartree

Product of the reaction for 4j:

Atom	x	y	z	Atom	x	y	z
C	-1.806335	-3.127265	0.233884	C	0.774094	2.767968	-0.228272
C	-0.543072	-2.631852	0.421155	C	2.101933	2.817989	0.048359
C	-0.279691	-1.246968	0.238917	C	3.029819	3.962922	0.048412
C	-1.350945	-0.380790	-0.141927	C	3.072735	4.843547	-1.039421
C	-2.650565	-0.929927	-0.327619	C	3.902487	4.161449	1.125600
C	-2.872854	-2.268266	-0.144667	C	3.960445	5.914347	-1.038587
H	-1.999753	-4.185737	0.374878	H	2.421638	4.675930	-1.891038
H	0.285302	-3.270114	0.710210	C	4.786968	5.235465	1.123567
N	0.989903	-0.798364	0.436561	H	3.874252	3.481600	1.972370
C	-1.080664	0.992263	-0.321301	C	4.816321	6.114999	0.043152
H	-3.458973	-0.264463	-0.616944	H	3.988848	6.588215	-1.888643
C	0.204542	1.445060	-0.126499	H	5.452025	5.385341	1.967720
C	1.187545	0.479531	0.256314	H	5.507916	6.951294	0.041446

H	-1.877716	1.673212	-0.609776	H	-3.866117	-2.680464	-0.288106
S	2.761272	1.233265	0.460961	I	-0.424433	4.407653	-0.668195

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.222664 hartree
Thermal correction to Gibbs free energy = 0.177756 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -7997.17173932 hartree

Reaction for 4k

Reactant1 of the reaction for 4k:

Atom	x	y	z	Atom	x	y	z
C	-1.902494	-2.453870	-1.724533	H	0.473337	6.320660	1.467501
C	-2.435256	-1.204768	-1.542720	C	3.551097	6.999605	2.749873
C	-1.659543	-0.181330	-0.940492	C	5.561166	5.517399	3.115128
C	-0.331990	-0.475373	-0.536959	H	5.859937	4.472756	3.001564
C	0.189341	-1.779880	-0.738883	H	6.255844	6.134731	2.536789
C	-0.571538	-2.764236	-1.321959	H	5.678494	5.793555	4.167644
C	0.416870	0.572464	0.041316	H	4.128352	7.825375	3.158200
C	-0.145538	1.822455	0.200195	N	-2.224322	1.046716	-0.756492
C	-1.515068	1.998523	-0.208794	S	-2.322734	3.589748	-0.060926
C	1.303478	3.803291	1.171174	C	2.242255	7.213511	2.327568
C	0.628506	2.900134	0.725711	C	-0.036851	-4.153599	-1.545177
H	-2.501771	-3.234691	-2.185828	H	0.992234	-4.244717	-1.190699
H	-3.449279	-0.965602	-1.846153	H	-0.648253	-4.894375	-1.019615
H	1.209138	-1.988618	-0.424198	H	-0.058170	-4.411925	-2.608916
H	1.446086	0.400534	0.343952	H	1.802319	8.202581	2.406700
C	2.067477	4.890664	1.703509	C	-2.292683	3.835642	1.743885
C	3.388390	4.686225	2.132069	H	-2.858802	4.750397	1.929568
C	1.493805	6.165126	1.803101	H	-1.274235	3.959464	2.112385
C	4.141143	5.733218	2.656875	H	-2.784753	3.003060	2.248064
H	3.822557	3.693745	2.050401				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.313796 hartree
Thermal correction to Gibbs free energy = 0.260948 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -1225.12831948 hartree

Entrance1 of the reaction for 4k:

Atom	x	y	z	Atom	x	y	z
C	-2.322356	-3.024928	-0.143233	C	2.853106	4.383424	-0.306471
C	-1.049916	-2.847360	0.333147	C	2.321277	5.510161	-0.952584
C	-0.396751	-1.599411	0.167730	C	4.126889	4.444910	0.273498

C	-1.084329	-0.548760	-0.492898	C	3.045995	6.696029	-1.029331
C	-2.400937	-0.766033	-0.975841	H	1.330285	5.449827	-1.393937
C	-3.023629	-1.979787	-0.810974	C	4.853893	5.628211	0.197162
H	-2.818214	-3.983415	-0.013799	H	4.529805	3.572306	0.777474
H	-0.512970	-3.641916	0.840626	C	4.318901	6.740055	-0.446641
N	0.875939	-1.458848	0.637762	H	5.841158	5.683376	0.644074
C	-0.412427	0.686022	-0.620332	H	4.894067	7.660843	-0.499336
H	-2.913536	0.050264	-1.478826	I	-0.690637	4.121764	1.005585
C	0.863457	0.833789	-0.115864	I	-2.888276	5.380325	1.960984
C	1.483246	-0.310091	0.500460	C	2.481242	7.910093	-1.721429
H	-0.909478	1.527539	-1.095377	H	1.478965	7.714838	-2.109525
S	3.129430	-0.199389	1.193885	H	2.421193	8.758573	-1.032784
C	4.111667	0.153171	-0.299390	H	3.118084	8.213465	-2.558332
H	3.865159	1.128421	-0.720538	C	-4.419944	-2.230570	-1.313839
H	5.154768	0.153544	0.022719	H	-5.083975	-2.513777	-0.490705
H	3.967529	-0.632174	-1.042306	H	-4.833168	-1.342981	-1.797906
C	1.527349	2.096129	-0.178396	H	-4.430708	-3.052921	-2.036614
C	2.105590	3.163845	-0.238835				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.314799 hartree
Thermal correction to Gibbs free energy = 0.250356 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15006.1099360 hartree

TS1 of the reaction for 4k:

Atom	x	y	z	Atom	x	y	z
C	0.000000	0.000000	0.000000	H	4.602400	-0.002430	1.558010
C	0.000000	0.000000	1.370251	H	3.105957	-2.257628	5.692703
C	1.227395	0.000000	2.078942	H	1.317291	-2.215820	5.784875
C	2.444306	0.000573	1.349260	H	2.297963	-1.936867	7.250428
C	2.408824	0.000990	-0.068496	C	5.840067	-1.331505	7.398999
C	1.213103	0.000662	-0.746828	C	5.657342	1.096795	7.624961
C	3.652224	-0.000701	2.084070	C	6.374297	-1.430048	8.677745
N	1.195752	0.001674	3.443796	C	6.537624	-0.250067	9.417963
C	3.616571	-0.000303	3.457056	C	6.185778	0.997418	8.903233
C	2.324964	-0.000724	4.093729	H	5.703092	-2.220915	6.790515
C	4.793014	-0.010473	4.308914	H	5.372975	2.054714	7.203678
C	4.946600	-0.006821	5.564134	C	6.776384	-2.759472	9.260477
C	5.485664	-0.075014	6.867440	H	6.951562	-0.313913	10.420965
I	6.910578	-0.062347	3.357717	H	6.326480	1.889620	9.503248
I	9.469321	-0.140230	1.803282	H	6.277689	-2.930651	10.218975
S	2.257452	0.010370	5.884081	H	6.519525	-3.580304	8.587593
C	2.243504	-1.788496	6.170586	H	7.855274	-2.791448	9.440796
H	-0.943315	0.000070	-0.539613	H	0.619850	0.882966	-2.617395
H	-0.921517	0.000268	1.942663	H	2.156206	0.000892	-2.686681
C	1.154990	0.001140	-2.250581	H	0.619032	-0.879922	-2.618035

H	3.349125	0.001679	-0.613948

Number of imaginary frequencies = 1 (-173.0858 cm^{-1})
Zero-point vibrational correction = 0.314501 hartree
Thermal correction to Gibbs free energy = 0.251109 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15006.0976873 hartree

IM of the reaction for 4k:

Atom	x	y	z	Atom	x	y	z
C	-2.402032	-2.577234	-2.039105	C	1.449106	7.374068	1.876086
C	-2.697937	-1.260713	-1.803524	C	2.598992	6.314529	3.858263
C	-1.693903	-0.388083	-1.318660	H	2.669266	5.343357	4.353017
C	-0.381431	-0.895554	-1.080125	H	3.616984	6.671121	3.671157
C	-0.116501	-2.264781	-1.339297	H	2.125441	7.020574	4.546614
C	-1.098268	-3.103751	-1.809935	H	1.711078	8.346476	2.284417
C	0.616511	-0.017597	-0.589351	N	-2.014059	0.924622	-1.100915
C	0.282749	1.294113	-0.352951	S	-1.285687	3.410391	-0.313247
C	-1.055343	1.656800	-0.646241	I	3.113071	2.127050	0.602659
C	0.411281	3.567871	0.292806	C	0.740696	7.295287	0.681634
C	1.080400	2.402761	0.166923	C	-0.830634	-4.557553	-2.088263
H	-3.174610	-3.244343	-2.411459	H	0.205917	-4.820136	-1.867603
H	-3.688760	-0.855867	-1.978927	H	-1.484664	-5.193176	-1.482811
H	0.886070	-2.642088	-1.156559	H	-1.030435	-4.792371	-3.138636
H	1.622706	-0.382274	-0.401147	H	0.455557	8.201488	0.157778
C	0.777580	4.887582	0.822983	C	-2.251305	3.377202	1.227015
C	1.477169	4.979330	2.033992	H	-3.260573	3.064674	0.956556
C	0.399102	6.055458	0.150649	H	-1.784743	2.682667	1.924919
C	1.827253	6.217323	2.567945	H	-2.254725	4.396900	1.614394
H	1.742346	4.071282	2.566853	I	6.458512	1.579375	1.252810
H	-0.136017	5.998176	-0.793173				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.317539 hartree
Thermal correction to Gibbs free energy = 0.258883 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15006.1330328 hartree

Reactant2 of the reaction for 4k:

Atom	x	y	z	Atom	x	y	z
C	-2.410820	-2.581154	-2.018455	H	-0.085785	5.997881	-0.821531
C	-2.705307	-1.265068	-1.778511	C	1.471249	7.369816	1.866397
C	-1.695495	-0.392318	-1.307226	C	2.555606	6.312284	3.885288
C	-0.379005	-0.899321	-1.086011	H	2.736300	5.324732	4.315341
C	-0.115823	-2.267639	-1.349840	H	3.521847	6.808137	3.750916
C	-1.103445	-3.106849	-1.807948	H	1.983615	6.901793	4.608120
C	0.623977	-0.021276	-0.607070	H	1.737770	8.341297	2.273906

C	0.289709	1.288968	-0.366043	N	-2.013027	0.919974	-1.085013
C	-1.050985	1.653085	-0.641886	S	-1.279933	3.407731	-0.307673
C	0.416122	3.572103	0.284490	I	3.093283	2.159664	0.552545
C	1.080026	2.405639	0.143286	C	0.783432	7.293556	0.660010
H	-3.187784	-3.248892	-2.380102	C	-0.838754	-4.559764	-2.091994
H	-3.698794	-0.861338	-1.940075	H	0.200868	-4.822230	-1.886407
H	0.889240	-2.644497	-1.180907	H	-1.484328	-5.196178	-1.478483
H	1.632285	-0.386639	-0.431976	H	-1.053652	-4.792618	-3.139770
C	0.790463	4.888056	0.815539	H	0.518842	8.200090	0.126399
C	1.469725	4.976176	2.038789	C	-2.234229	3.381687	1.240276
C	0.435298	6.055154	0.129896	H	-3.245770	3.073136	0.973479
C	1.821859	6.212958	2.573275	H	-1.767285	2.685361	1.935847
H	1.712477	4.068732	2.583927	H	-2.231640	4.402667	1.624033

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.317316 hartree
Thermal correction to Gibbs free energy = 0.264737 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8115.46656808 hartree

Entrance2 of the reaction for 4k:

Atom	x	y	z	Atom	x	y	z
C	-2.406417	-2.578742	-2.039779	C	1.489879	7.367734	1.836351
C	-2.699332	-1.262168	-1.801683	C	2.493937	6.314631	3.898617
C	-1.690444	-0.390318	-1.325549	H	2.691299	5.326373	4.319565
C	-0.376033	-0.899193	-1.099138	H	3.447132	6.843553	3.803012
C	-0.114256	-2.268572	-1.360825	H	1.879650	6.872529	4.612012
C	-1.101047	-3.106537	-1.822171	H	1.760117	8.339013	2.241986
C	0.626024	-0.021648	-0.617635	N	-2.009197	0.921054	-1.102351
C	0.291491	1.288553	-0.377871	S	-1.285264	3.403023	-0.302711
C	-1.049186	1.655707	-0.654852	I	3.094596	2.164613	0.543906
C	0.415801	3.571551	0.265418	C	0.831530	7.290466	0.613601
C	1.080972	2.405812	0.129223	C	-0.838409	-4.561148	-2.100626
H	-3.183208	-3.245551	-2.403654	H	0.200574	-4.824556	-1.892540
H	-3.691760	-0.856760	-1.965755	H	-1.485333	-5.194157	-1.484937
H	0.889151	-2.647420	-1.185922	H	-1.052428	-4.798494	-3.147621
H	1.633538	-0.387408	-0.438602	H	0.593762	8.196025	0.065797
C	0.796874	4.887580	0.792678	C	-2.212630	3.350792	1.281469
C	1.446860	4.976552	2.031170	H	-3.230765	3.048706	1.038017
C	0.476114	6.052493	0.087268	H	-1.730574	2.642588	1.952457
C	1.802714	6.213094	2.563849	H	-2.198498	4.361480	1.688108
H	1.658515	4.070044	2.590856	I	-3.925325	3.289066	4.267525
H	-0.026584	5.992018	-0.873712				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.317205 hartree
Thermal correction to Gibbs free energy = 0.257056 hartree

M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15006.1336824 hartree

TS2 of the reaction for 4k:

Atom	x	y	z	Atom	x	y	z
C	-2.406988	-2.548117	-2.092750	C	1.503885	7.380039	1.789056
C	-2.690083	-1.228501	-1.865610	C	2.434770	6.343150	3.893639
C	-1.687255	-0.363271	-1.357802	H	2.616615	5.357818	4.328518
C	-0.388137	-0.890481	-1.088484	H	3.392771	6.866753	3.818634
C	-0.135856	-2.265772	-1.339317	H	1.805413	6.910241	4.586609
C	-1.115107	-3.092439	-1.831762	H	1.780669	8.353268	2.185765
C	0.606248	-0.025114	-0.577324	N	-2.001038	0.948127	-1.148510
C	0.282076	1.292577	-0.356485	S	-1.275085	3.415824	-0.333340
C	-1.045766	1.688168	-0.678101	I	3.067302	2.141410	0.644010
C	0.401935	3.573980	0.247470	C	0.876188	7.292400	0.550993
C	1.067941	2.399692	0.161834	C	-0.861366	-4.550876	-2.100688
H	-3.179663	-3.205786	-2.481729	H	0.167670	-4.826103	-1.860033
H	-3.671713	-0.811346	-2.063210	H	-1.533758	-5.176787	-1.505147
H	0.857108	-2.655957	-1.131036	H	-1.044578	-4.788152	-3.153629
H	1.602509	-0.402740	-0.362222	H	0.667980	8.192571	-0.017673
C	0.797109	4.892200	0.765609	C	-2.293253	3.282282	1.585203
C	1.415996	4.992956	2.018724	H	-3.234972	2.916157	1.199266
C	0.514058	6.051231	0.035759	H	-1.607207	2.580459	2.040357
C	1.777667	6.232100	2.542121	H	-2.210224	4.330128	1.839306
H	1.599018	4.092054	2.597423	I	-3.592844	3.127464	4.075437
H	0.033804	5.980770	-0.935937				

Number of imaginary frequencies = 1 (-491.6115 cm^{-1})
Zero-point vibrational correction = 0.316050 hartree
Thermal correction to Gibbs free energy = 0.257032 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15006.1254332 hartree

Product of the reaction for 4k:

Atom	x	y	z	Atom	x	y	z
C	-2.396686	-2.562002	-2.096066	C	1.804195	6.237438	2.540448
C	-2.698571	-1.254540	-1.833519	H	1.604210	4.101844	2.646854
C	-1.709321	-0.379422	-1.305556	H	-0.083323	5.933157	-0.853950
C	-0.400956	-0.894981	-1.057665	C	1.512845	7.374269	1.777736
C	-0.128575	-2.262267	-1.345364	C	2.531390	6.364422	3.854769
C	-1.093623	-3.092705	-1.853839	H	2.603052	5.400017	4.363036
C	0.578335	-0.025859	-0.533903	H	3.547232	6.743207	3.702139
C	0.234502	1.283389	-0.278858	H	2.018772	7.065312	4.520683
C	-1.107554	1.677137	-0.572986	H	1.816871	8.351951	2.142759
C	0.308154	3.545669	0.349279	N	-2.049538	0.913615	-1.058975
C	1.006519	2.386732	0.241906	S	-1.364110	3.372055	-0.187395
H	-3.160369	-3.222041	-2.499373	I	3.028154	2.161124	0.669310

H	-3.688219	-0.849093	-2.016985	C	0.834932	7.267118	0.568055
H	0.872487	-2.640480	-1.151589	C	-0.817450	-4.540081	-2.161454
H	1.583557	-0.389831	-0.335863	H	0.216413	-4.804992	-1.928716
C	0.733449	4.870442	0.834910	H	-1.478002	-5.194064	-1.582629
C	1.405892	4.992654	2.057677	H	-0.996742	-4.754324	-3.220227
C	0.438458	6.019253	0.094620	H	0.613565	8.157743	-0.011131

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.278216 hartree
Thermal correction to Gibbs free energy = 0.228429 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8075.78669842 hartree

Reaction for 4l

Reactant1 of the reaction for 4l:

Atom	x	y	z	Atom	x	y	z
C	-1.925989	-2.766291	-1.456374	H	2.984814	5.072578	-0.895864
C	-2.520704	-1.721963	-0.788402	C	2.276146	8.140970	0.359472
C	-1.846585	-0.487219	-0.614649	H	0.436053	8.693545	1.325053
C	-0.539050	-0.326517	-1.141257	H	2.718585	9.127016	0.476622
C	0.065235	-1.412325	-1.828256	N	-2.478971	0.507822	0.073556
C	-0.611514	-2.593050	-1.978221	S	-2.807188	2.912903	1.104381
C	0.087896	0.924336	-0.964005	C	-2.627157	-4.084371	-1.647525
C	-0.565274	1.939022	-0.293929	H	-2.727323	-4.319668	-2.712140
C	-1.873474	1.655044	0.236080	H	-2.055648	-4.897847	-1.188640
C	0.555910	4.318253	-0.075245	H	-3.624521	-4.071679	-1.202905
C	0.034963	3.227516	-0.168779	H	-0.145663	-3.421574	-2.505203
H	-3.520388	-1.814891	-0.374094	C	4.397552	7.412539	-0.798542
H	1.066352	-1.288382	-2.231488	H	4.359488	8.106689	-1.644453
H	1.079181	1.097059	-1.373845	H	5.023621	7.871855	-0.027767
C	1.138864	5.618049	0.067256	H	4.887017	6.496037	-1.136137
C	0.415637	6.640916	0.695386	C	-1.726619	3.233193	2.535409
C	2.433111	5.873535	-0.411795	H	-0.785705	3.691540	2.230647
C	0.991583	7.898579	0.837712	H	-2.277005	3.926341	3.174506
H	-0.586100	6.440677	1.062349	H	-1.543122	2.309771	3.085982
C	3.012534	7.132001	-0.272993				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.313801 hartree
Thermal correction to Gibbs free energy = 0.261347 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -1225.12859621 hartree

Entrance1 of the reaction for 4l:

Atom	x	y	z	Atom	x	y	z
C	-2.334308	-3.047156	-0.140321	C	2.323358	5.512121	-0.953703
C	-1.058528	-2.843300	0.330928	C	4.127939	4.446946	0.273790
C	-0.408283	-1.595537	0.161245	C	3.047962	6.698112	-1.029573
C	-1.086690	-0.540654	-0.502800	H	1.332752	5.451779	-1.395941
C	-2.402971	-0.763268	-0.986361	C	4.854855	5.630374	0.198295
C	-3.003263	-1.980816	-0.807965	H	4.530582	3.574413	0.778117
H	-0.514532	-3.631233	0.843379	C	4.320359	6.742280	-0.445783
N	0.864669	-1.456116	0.634039	H	5.841703	5.685563	0.646139
C	-0.413046	0.691382	-0.630653	H	4.895438	7.663160	-0.497806
H	-2.921583	0.045245	-1.493338	H	-4.011186	-2.147522	-1.178210
C	0.862261	0.836987	-0.122733	I	-0.682089	4.120830	1.014077
C	1.475007	-0.308979	0.495943	I	-2.877633	5.377751	1.977104
H	-0.907167	1.533189	-1.108329	C	2.483603	7.912208	-1.721954
S	3.120161	-0.204498	1.193459	H	1.481670	7.716878	-2.110903
C	4.107233	0.156309	-0.294645	H	2.422875	8.760590	-1.033244
H	3.867980	1.136816	-0.707502	H	3.121083	8.215809	-2.558293
H	5.149542	0.146819	0.029869	C	-3.039244	-4.365713	0.030675
H	3.959936	-0.621361	-1.044977	H	-2.412397	-5.085804	0.560804
C	1.528593	2.097850	-0.182809	H	-3.969239	-4.237385	0.594115
C	2.107065	3.165659	-0.240946	H	-3.306245	-4.791229	-0.942220
C	2.854719	4.385247	-0.307390				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.314772 hartree
Thermal correction to Gibbs free energy = 0.250346 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15006.1102444 hartree

TS1 of the reaction for 4l:

Atom	x	y	z	Atom	x	y	z
C	0.000000	0.000000	0.000000	H	4.602765	-0.002271	1.656542
C	0.000000	0.000000	1.375398	H	3.008549	-2.262249	5.750851
C	1.215098	0.000000	2.102878	H	1.218368	-2.214041	5.802580
C	2.450644	0.000831	1.404460	H	2.166594	-1.943397	7.290966
C	2.437404	0.001292	-0.014643	C	5.705821	-1.333582	7.529698
C	1.246154	0.000721	-0.690303	C	5.531785	1.096391	7.743914
C	3.641884	-0.000459	2.162865	C	6.210706	-1.430922	8.820366
N	1.155777	0.001440	3.468120	C	6.364850	-0.249348	9.560097
C	3.577120	-0.000339	3.535366	C	6.031753	0.998393	9.033722
C	2.271340	-0.000920	4.141105	H	5.577402	-2.224238	6.921191
C	4.734034	-0.011222	4.413031	H	5.262376	2.054503	7.313333
C	4.860069	-0.009433	5.671497	C	6.590005	-2.760799	9.417161
C	5.370148	-0.076916	6.986429	H	6.756462	-0.312223	10.572093
I	6.870770	-0.058117	3.508142	H	6.164737	1.891837	9.633651
I	9.465196	-0.127537	2.010636	H	6.053704	-2.932845	10.355068
S	2.164337	0.008076	5.930239	H	6.359566	-3.581049	8.734099

C	2.137182	-1.791532	6.210653	H	7.660840	-2.792980	9.640099
C	-1.280235	0.000015	-0.790535	H	-2.152847	-0.001129	-0.134064
H	-0.927905	0.000193	1.939307	H	-1.335462	0.882026	-1.436805
H	1.240607	0.001003	-1.776849	H	-1.334428	-0.880650	-1.438740
H	3.382102	0.002120	-0.550260				

Number of imaginary frequencies = 1 (-171.8180 cm^{-1})
Zero-point vibrational correction = 0.314587 hartree
Thermal correction to Gibbs free energy = 0.253083 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15006.0979420 hartree

IM of the reaction for 4l:

Atom	x	y	z	Atom	x	y	z
C	-1.970618	-3.057287	-1.163220	C	0.884085	7.545783	1.852581
C	-2.153024	-2.022177	-0.276290	H	-1.226930	7.792881	2.182245
C	-1.506116	-0.779303	-0.470294	H	1.134885	8.526191	2.248310
C	-0.650816	-0.589862	-1.597274	N	-1.730459	0.221502	0.438574
C	-0.477594	-1.670256	-2.502410	S	-1.282850	2.750915	1.293976
C	-1.117636	-2.860995	-2.287281	I	1.606080	3.729892	-2.245970
C	-0.004134	0.655862	-1.775240	C	-2.648662	-4.386461	-0.976085
C	-0.217693	1.647667	-0.847635	H	-3.277685	-4.622733	-1.840276
C	-1.100030	1.322775	0.211783	H	-1.907696	-5.187231	-0.885401
C	-0.092215	3.702433	0.320733	H	-3.274364	-4.391660	-0.081409
C	0.324419	3.000977	-0.754365	H	-0.978516	-3.681965	-2.985031
H	-2.796140	-2.129572	0.591681	C	3.343699	7.169455	1.414487
H	0.169709	-1.533432	-3.363199	H	4.030924	6.322326	1.355098
H	0.651067	0.817509	-2.626975	H	3.550656	7.826132	0.562901
C	0.233396	5.037092	0.840067	H	3.562717	7.732178	2.325879
C	-0.777179	5.881055	1.316490	C	-0.300318	2.248162	2.739033
C	1.569406	5.454463	0.894766	H	0.666029	1.874720	2.401376
C	-0.444919	7.134581	1.818934	H	-0.193268	3.132904	3.368022
H	-1.817637	5.571309	1.273945	H	-0.875972	1.477733	3.253376
C	1.908395	6.712301	1.390071	I	3.704280	4.846098	-4.747783
H	2.352284	4.783783	0.554064				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.317319 hartree
Thermal correction to Gibbs free energy = 0.257789 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15006.1332266 hartree

Reactant2 of the reaction for 4l:

Atom	x	y	z	Atom	x	y	z
C	-1.960644	-3.063907	-1.137168	H	2.351026	4.752942	0.613941
C	-2.135900	-2.026266	-0.251302	C	0.879353	7.570034	1.785996
C	-1.496040	-0.782591	-0.458415	H	-1.237885	7.864282	2.018781

C	-0.654859	-0.594294	-1.597179	H	1.131430	8.555690	2.167774
C	-0.488610	-1.677100	-2.500437	N	-1.713295	0.221385	0.448578
C	-1.122216	-2.868851	-2.272473	S	-1.271424	2.757013	1.289831
C	-0.016498	0.653198	-1.788330	I	1.541843	3.749038	-2.248396
C	-0.224942	1.646019	-0.861356	C	-2.631520	-4.394405	-0.937386
C	-1.091501	1.324019	0.211160	H	-3.264951	-4.637929	-1.796225
C	-0.102287	3.713548	0.305056	H	-1.886013	-5.190994	-0.847513
C	0.300742	3.004157	-0.769677	H	-3.250896	-4.397052	-0.038492
H	-2.767839	-2.132613	0.624817	H	-0.989480	-3.692061	-2.968704
H	0.147248	-1.541877	-3.369937	C	3.348755	7.137941	1.491487
H	0.626684	0.813465	-2.649417	H	3.544684	7.989128	0.831904
C	0.226129	5.053188	0.807114	H	3.590907	7.452177	2.511079
C	-0.789120	5.922203	1.221473	H	4.026250	6.328281	1.211608
C	1.567777	5.446661	0.905886	C	-0.268030	2.273288	2.727845
C	-0.454164	7.182722	1.706110	H	0.696063	1.901122	2.382821
H	-1.831738	5.627396	1.143331	H	-0.161146	3.163844	3.348624
C	1.908647	6.707388	1.389651	H	-0.836023	1.504182	3.252708

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.317380 hartree
Thermal correction to Gibbs free energy = 0.265092 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8115.46708625 hartree

Entrance2 of the reaction for 4l:

Atom	x	y	z	Atom	x	y	z
C	6.082637	0.448190	0.293068	C	-5.125073	-1.239416	1.353570
C	4.912468	0.823947	0.910044	H	-4.739214	-1.166018	3.467694
C	3.706805	0.126959	0.662661	H	-6.203524	-1.287651	1.478306
C	3.696618	-0.981222	-0.237652	N	2.572442	0.539089	1.310015
C	4.915635	-1.354277	-0.863063	S	-0.076137	0.273888	1.794108
C	6.065811	-0.659388	-0.603116	I	-0.527226	-3.358117	-1.039250
C	2.482700	-1.665868	-0.478758	C	7.375187	1.175776	0.540212
C	1.346568	-1.231392	0.160580	H	8.131218	0.492600	0.940383
C	1.503575	-0.125613	1.032457	H	7.770258	1.585683	-0.394802
C	-0.912746	-1.020441	0.862300	H	7.241159	1.996437	1.247541
C	-0.031494	-1.705926	0.104895	H	6.993361	-0.951087	-1.087706
H	4.881148	1.661647	1.599663	C	-5.489914	-1.298779	-1.143296
H	4.916785	-2.195466	-1.549374	H	-6.058971	-2.233717	-1.154550
H	2.457197	-2.512079	-1.160314	H	-6.211259	-0.476301	-1.130001
C	-2.366810	-1.113392	1.041870	H	-4.917934	-1.236674	-2.071626
C	-2.922363	-1.099197	2.325813	C	-0.567198	1.788918	0.880970
C	-3.202967	-1.171061	-0.081405	H	-0.444407	1.615916	-0.186663
C	-4.304130	-1.168133	2.474026	H	-1.606241	1.990707	1.139967
H	-2.281254	-1.055667	3.201635	H	0.078874	2.590360	1.237445
C	-4.586737	-1.238537	0.061036	I	-1.458604	4.706737	-0.709498
H	-2.766429	-1.143857	-1.075667				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.317166 hartree
Thermal correction to Gibbs free energy = 0.256586 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15006.1341057 hartree

TS2 of the reaction for 4l:

Atom	x	y	z	Atom	x	y	z
C	6.084818	0.059882	0.356499	C	-5.198991	-0.858283	1.471024
C	4.951294	0.488878	1.003312	H	-4.778916	-0.911208	3.579096
C	3.688814	-0.093580	0.728552	H	-6.276702	-0.849760	1.611267
C	3.590207	-1.142350	-0.235555	N	2.598309	0.372947	1.405968
C	4.775282	-1.573220	-0.892093	S	-0.056364	0.306868	1.879078
C	5.977962	-0.989491	-0.603174	I	-0.814349	-3.123126	-1.137043
C	2.325882	-1.709785	-0.507253	C	7.431888	0.669064	0.633838
C	1.229432	-1.226793	0.168467	H	8.135758	-0.092746	0.984317
C	1.467723	-0.189146	1.110874	H	7.853033	1.104554	-0.278118
C	-0.982674	-0.877176	0.922819	H	7.365670	1.452778	1.391193
C	-0.176590	-1.586677	0.099791	H	6.877855	-1.324645	-1.111451
H	4.990073	1.284979	1.740544	C	-5.599781	-0.768630	-1.019502
H	4.705807	-2.370756	-1.625828	H	-6.292448	-1.615879	-1.017052
H	2.229106	-2.507130	-1.239786	H	-6.201288	0.145551	-1.002293
C	-2.439928	-0.886267	1.118978	H	-5.038497	-0.788682	-1.956306
C	-2.977285	-0.899021	2.410286	C	-0.450839	2.090494	0.699126
C	-3.295168	-0.837540	0.010206	H	-0.309378	1.625909	-0.267189
C	-4.358802	-0.890673	2.579014	H	-1.459177	2.260824	1.051755
H	-2.320564	-0.936359	3.274726	H	0.349586	2.688771	1.112882
C	-4.678687	-0.826719	0.171693	I	-0.929667	4.375691	-0.872913
H	-2.870756	-0.790446	-0.988491				

Number of imaginary frequencies = 1 (-490.7209 cm^{-1})
Zero-point vibrational correction = 0.315978 hartree
Thermal correction to Gibbs free energy = 0.256609 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15006.1255042 hartree

Product of the reaction for 4l:

Atom	x	y	z	Atom	x	y	z
C	-1.974798	-3.044084	-1.186658	H	-1.789367	5.529270	1.194966
C	-2.113184	-2.022222	-0.281780	C	1.906697	6.758384	1.257906
C	-1.451758	-0.777244	-0.465523	H	2.391416	4.795651	0.533045
C	-0.626649	-0.590683	-1.616402	C	0.864999	7.598551	1.666462
C	-0.497196	-1.663524	-2.543885	H	-1.251776	7.820362	1.971964
C	-1.148702	-2.846127	-2.334228	H	1.095352	8.604367	2.008003
C	0.027509	0.644804	-1.790898	N	-1.633050	0.195147	0.468496
C	-0.150983	1.628029	-0.842574	S	-1.118485	2.686152	1.362604

C	-1.004791	1.322111	0.261543	I	1.571879	3.745055	-2.262467
C	-0.042747	3.650150	0.347614	C	-2.670619	-4.365583	-1.001218
C	0.372491	2.970335	-0.751524	H	-3.336002	-4.575411	-1.845246
H	-2.733046	-2.135271	0.602858	H	-1.943859	-5.183180	-0.951644
H	0.129401	-1.521559	-3.419987	H	-3.264167	-4.377092	-0.084502
H	0.660645	0.811989	-2.658826	H	-1.043350	-3.658534	-3.048195
C	0.267277	5.020045	0.793296	C	3.334107	7.242553	1.274553
C	-0.758662	5.870636	1.217695	H	3.513832	7.946719	0.455137
C	1.592961	5.470068	0.828838	H	3.562814	7.763149	2.208889
C	-0.454655	7.158720	1.648688	H	4.035565	6.412422	1.162247

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.278232 hartree
Thermal correction to Gibbs free energy = 0.228446 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8075.78710277 hartree

Reaction for 4m

Reactant1 of the reaction for 4m:

Atom	x	y	z	Atom	x	y	z
C	-1.765997	-3.075296	-1.929577	C	0.198129	6.192162	0.972794
C	-2.322080	-1.840382	-2.153535	C	2.412498	6.113020	2.708625
C	-1.793519	-0.695581	-1.506493	H	2.352667	3.982838	2.411732
C	-0.685807	-0.841412	-0.630514	C	0.708132	7.367446	1.513773
C	-0.130966	-2.129400	-0.415358	H	-0.652651	6.210733	0.298934
C	-0.661673	-3.222189	-1.052792	C	1.802963	7.327923	2.372240
C	-0.178086	0.328247	-0.022805	C	3.598386	6.086605	3.639210
C	-0.757113	1.552553	-0.282482	H	3.961797	5.067453	3.789732
C	-1.903104	1.580147	-1.156307	H	4.421838	6.686584	3.239363
C	0.270154	3.752776	0.751262	H	3.336777	6.502945	4.617110
C	-0.208771	2.745783	0.275606	H	2.195220	8.251885	2.789678
H	-2.172449	-3.950926	-2.425397	N	-2.383139	0.514087	-1.738972
H	-3.168815	-1.704382	-2.818204	S	-2.707374	3.125217	-1.571296
H	0.716411	-2.231102	0.256669	H	0.249799	8.318993	1.263644
H	-0.236952	-4.207131	-0.888766	C	-3.297388	3.669952	0.063861
H	0.684488	0.266326	0.634792	H	-3.936181	2.906764	0.509941
C	0.794382	4.966872	1.299528	H	-2.467403	3.911786	0.727777
C	1.898351	4.938513	2.165846	H	-3.889313	4.569009	-0.118176

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.286088 hartree
Thermal correction to Gibbs free energy = 0.236162 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -1185.82054612 hartree

Entrance1 of the reaction for 4m:

Atom	x	y	z	Atom	x	y	z
C	-2.327028	-3.031758	-0.147909	C	1.525579	2.096468	-0.174420
C	-1.051904	-2.850089	0.327505	C	2.103911	3.164351	-0.229595
C	-0.403847	-1.600851	0.161292	C	2.850166	4.384944	-0.291383
C	-1.088463	-0.545116	-0.496941	C	2.317008	5.513759	-0.932781
C	-2.405152	-0.759625	-0.979781	C	4.123572	4.445463	0.289484
C	-3.009918	-1.979034	-0.807700	C	3.040088	6.700961	-1.003774
H	-2.821609	-3.989121	-0.020228	H	1.326357	5.453918	-1.374972
H	-0.509950	-3.641862	0.833760	C	4.848988	5.630073	0.218718
N	0.870910	-1.461196	0.630504	H	4.527481	3.571200	0.789782
C	-0.414844	0.689790	-0.621422	C	4.312708	6.744028	-0.420355
H	-2.920510	0.054656	-1.480617	H	5.836017	5.684584	0.666211
C	0.860694	0.834549	-0.117633	H	4.886681	7.665794	-0.468742
C	1.479001	-0.313629	0.495016	H	-4.017116	-2.143453	-1.175806
H	-0.911842	1.532923	-1.093621	I	-0.690570	4.116430	1.029449
S	3.125857	-0.208151	1.187422	I	-2.887678	5.368262	1.993897
C	4.107236	0.159157	-0.302935	C	2.473741	7.917609	-1.690002
H	3.864613	1.140290	-0.712237	H	1.474832	7.720543	-2.085782
H	5.150483	0.151034	0.018536	H	2.405203	8.760302	-0.995050
H	3.959409	-0.616814	-1.054894	H	3.114321	8.230657	-2.520424

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.287039 hartree
Thermal correction to Gibbs free energy = 0.224740 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8020325 hartree

TS1 of the reaction for 4m:

Atom	x	y	z	Atom	x	y	z
C	0.008906	-0.046181	0.008574	H	1.198462	0.038408	-1.801541
C	0.013535	-0.073084	1.381323	H	3.364042	0.100881	-0.605647
C	1.242267	-0.037965	2.084740	H	4.618326	0.097475	1.570790
C	2.461565	0.024520	1.359327	H	3.179053	-2.300663	5.658704
C	2.427639	0.052126	-0.058009	H	1.389361	-2.306922	5.742275
C	1.224512	0.017422	-0.717258	H	2.355634	-2.032904	7.218362
C	3.668659	0.053569	2.095981	C	5.889761	-1.307054	7.391748
N	1.211514	-0.063243	3.451187	C	5.638045	1.111534	7.653616
C	3.632040	0.024355	3.467776	C	6.430969	-1.408564	8.667302
C	2.339124	-0.035305	4.101270	C	6.562754	-0.235202	9.424140
C	4.806656	0.036806	4.321818	C	6.173252	1.008934	8.928818
C	4.955971	0.019060	5.577607	H	5.776308	-2.191234	6.770951
C	5.497989	-0.053634	6.879508	H	5.325169	2.066941	7.247082
I	6.925743	0.072949	3.374034	C	6.874706	-2.733768	9.228983
I	9.487833	0.118655	1.824720	H	6.981909	-0.301663	10.424796
S	2.270626	-0.059984	5.892026	H	6.290235	1.896069	9.541292
C	2.302449	-1.864045	6.141497	H	6.392589	-2.929383	10.191245

H	-0.932259	-0.073184	-0.530573	H	7.956246	-2.739155	9.395921
H	-0.903913	-0.120630	1.958050	H	6.631595	-3.553100	8.549199

Number of imaginary frequencies = 1 (-174.4995 cm^{-1})
Zero-point vibrational correction = 0.286838 hartree
Thermal correction to Gibbs free energy = 0.227896 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.7893184 hartree

IM of the reaction for 4m:

Atom	x	y	z	Atom	x	y	z
C	-2.445617	-2.632116	-1.904755	C	1.725172	6.237570	2.621874
C	-2.719847	-1.299001	-1.727086	H	1.580871	4.094784	2.697538
C	-1.720175	-0.436465	-1.219146	C	0.782497	7.265019	0.632597
C	-0.431112	-0.957882	-0.893030	H	-0.039724	5.932486	-0.841505
C	-0.182304	-2.340475	-1.091158	C	1.419837	7.373811	1.865330
C	-1.168330	-3.156416	-1.585070	C	2.431072	6.358456	3.947303
C	0.558338	-0.082626	-0.379543	H	2.220838	5.499062	4.588433
C	0.240720	1.242169	-0.206129	H	3.515340	6.404687	3.800301
C	-1.073305	1.618710	-0.582771	H	2.129263	7.267701	4.473580
C	0.381569	3.534557	0.366077	H	1.680435	8.355170	2.252072
C	1.032019	2.353296	0.318121	N	-2.022141	0.891230	-1.062053
H	-3.210981	-3.294537	-2.294734	S	-1.285544	3.387709	-0.320566
H	-3.688671	-0.874475	-1.966409	I	3.028467	2.050408	0.884020
H	0.798199	-2.735450	-0.844201	H	0.552199	8.156864	0.059503
H	-0.973153	-4.212865	-1.734128	C	-2.326593	3.419208	1.170052
H	1.545017	-0.460563	-0.125528	H	-3.323304	3.101882	0.861113
C	0.748047	4.865233	0.868061	H	-1.900894	2.749758	1.916918
C	1.374463	4.987352	2.114550	H	-2.341845	4.452847	1.518102
C	0.441187	6.014690	0.129170	I	6.304195	1.432699	1.768710

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.289654 hartree
Thermal correction to Gibbs free energy = 0.233088 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8248378 hartree

Reactant2 of the reaction for 4m:

Atom	x	y	z	Atom	x	y	z
C	-2.465674	-2.633052	-1.880299	C	1.715278	6.228247	2.630281
C	-2.735761	-1.299471	-1.699145	H	1.525787	4.090315	2.720911
C	-1.727814	-0.439428	-1.204771	C	0.860846	7.256661	0.600209
C	-0.434805	-0.963406	-0.895845	H	0.053643	5.925343	-0.885867
C	-0.190703	-2.346083	-1.097327	C	1.460707	7.363130	1.850536
C	-1.185181	-3.159735	-1.577930	C	2.353664	6.361970	3.988254
C	0.562638	-0.090056	-0.395809	H	2.441706	5.392476	4.483407
C	0.246943	1.234149	-0.218473	H	3.355817	6.793407	3.903011

C	-1.070585	1.614852	-0.575936	H	1.766418	7.024363	4.631305
C	0.390712	3.536482	0.354499	H	1.732157	8.342272	2.235752
C	1.034564	2.352379	0.291838	N	-2.024947	0.888598	-1.043122
H	-3.237203	-3.294228	-2.259843	S	-1.277950	3.385578	-0.313590
H	-3.706957	-0.873435	-1.925264	I	3.014935	2.080276	0.824906
H	0.792023	-2.743393	-0.863711	H	0.669771	8.147163	0.011129
H	-0.994339	-4.216514	-1.729700	C	-2.303572	3.429317	1.188081
H	1.551772	-0.470846	-0.155926	H	-3.302307	3.110008	0.887537
C	0.768775	4.862577	0.856827	H	-1.872647	2.764570	1.935966
C	1.358730	4.981396	2.122714	H	-2.316131	4.466309	1.526137
C	0.506957	6.008337	0.097737				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.289560 hartree
Thermal correction to Gibbs free energy = 0.239304 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8076.15821437 hartree

Entrance2 of the reaction for 4m:

Atom	x	y	z	Atom	x	y	z
C	-2.462780	-2.627263	-1.892859	C	1.721433	6.230942	2.617155
C	-2.729667	-1.292988	-1.713603	H	1.516047	4.094560	2.718014
C	-1.721691	-0.434500	-1.215314	C	0.893103	7.253220	0.573378
C	-0.431990	-0.962018	-0.900460	H	0.085879	5.917935	-0.910019
C	-0.190770	-2.345693	-1.100281	C	1.482660	7.362821	1.828339
C	-1.184831	-3.157204	-1.584853	C	2.338268	6.368741	3.984722
C	0.564997	-0.090630	-0.396499	H	2.489124	5.393353	4.452341
C	0.251078	1.234032	-0.221134	H	3.307021	6.874029	3.924489
C	-1.064490	1.620391	-0.583711	H	1.697512	6.965941	4.640759
C	0.396293	3.535627	0.345608	H	1.756611	8.342438	2.210765
C	1.039156	2.350928	0.288806	N	-2.017427	0.893536	-1.055437
H	-3.235085	-3.286741	-2.273926	S	-1.274093	3.386124	-0.311655
H	-3.699306	-0.864480	-1.941870	I	3.019122	2.077711	0.826337
H	0.789714	-2.745470	-0.861042	H	0.712513	8.141740	-0.022079
H	-0.996213	-4.214771	-1.734395	C	-2.298628	3.418689	1.212390
H	1.552082	-0.473331	-0.151175	H	-3.302250	3.113219	0.918712
C	0.781548	4.861603	0.843507	H	-1.868514	2.739566	1.946212
C	1.362159	4.983447	2.113084	H	-2.300291	4.448660	1.568144
C	0.534048	6.004492	0.075664	I	-4.302732	3.493510	4.007361

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.289476 hartree
Thermal correction to Gibbs free energy = 0.231257 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8254069 hartree

TS2 of the reaction for 4m:

Atom	x	y	z	Atom	x	y	z
C	-2.469463	-2.587907	-1.953189	C	1.693248	6.254132	2.593299
C	-2.718980	-1.248577	-1.796695	H	1.448871	4.123169	2.720173
C	-1.719873	-0.398352	-1.260261	C	0.944925	7.256285	0.510535
C	-0.455895	-0.948221	-0.884305	H	0.157270	5.908080	-0.973713
C	-0.231938	-2.339724	-1.061045	C	1.498330	7.377427	1.780777
C	-1.215628	-3.138767	-1.582846	C	2.274052	6.402345	3.975799
C	0.530807	-0.090529	-0.344459	H	2.369732	5.433979	4.471918
C	0.234794	1.243321	-0.198997	H	3.265285	6.864350	3.933358
C	-1.057825	1.661475	-0.623006	H	1.641020	7.043046	4.597448
C	0.382935	3.542870	0.323439	H	1.778347	8.358294	2.155829
C	1.018409	2.348705	0.326395	N	-2.003727	0.931235	-1.123689
H	-3.235803	-3.236875	-2.363710	S	-1.258463	3.407178	-0.356829
H	-3.669722	-0.805413	-2.072503	I	2.973058	2.055127	0.950689
H	0.729919	-2.753688	-0.773855	H	0.797603	8.137907	-0.104339
H	-1.039610	-4.200951	-1.714763	C	-2.397262	3.343856	1.492613
H	1.498385	-0.487876	-0.048914	H	-3.313628	2.965219	1.060259
C	0.783362	4.870028	0.813416	H	-1.745158	2.657301	2.015644
C	1.327665	5.004891	2.097457	H	-2.329987	4.398926	1.719965
C	0.578987	6.005257	0.022556	I	-3.854438	3.254641	3.901029

Number of imaginary frequencies = 1 (-488.8093 cm^{-1})
Zero-point vibrational correction = 0.288387 hartree
Thermal correction to Gibbs free energy = 0.231954 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -14966.8172970 hartree

Product of the reaction for 4m:

Atom	x	y	z	Atom	x	y	z
C	-2.435413	-2.610505	-1.987010	C	1.317147	4.995139	2.133612
C	-2.713027	-1.284181	-1.786692	C	0.479787	5.973417	0.087841
C	-1.731955	-0.420717	-1.227788	C	1.716593	6.247193	2.595915
C	-0.453806	-0.956326	-0.878252	H	1.464138	4.120855	2.761092
C	-0.200048	-2.338735	-1.100595	C	0.878402	7.228307	0.540471
C	-1.165427	-3.145195	-1.640835	H	0.009002	5.865691	-0.884865
C	0.513659	-0.092498	-0.322843	C	1.493188	7.362838	1.780690
C	0.189433	1.232087	-0.135646	C	2.364899	6.405890	3.947512
C	-1.121518	1.646638	-0.529657	H	2.502561	5.439050	4.437170
C	0.282346	3.513087	0.416212	H	3.344696	6.884988	3.856444
C	0.955687	2.334716	0.395436	H	1.754023	7.035229	4.602579
H	-3.189505	-3.263598	-2.414168	H	1.800931	8.345707	2.128278
H	-3.675904	-0.855365	-2.043919	N	-2.050880	0.890007	-1.047699
H	0.774135	-2.737615	-0.832386	S	-1.356865	3.359931	-0.220999
H	-0.965306	-4.198364	-1.807710	I	2.937603	2.071796	0.963394
H	1.494160	-0.474050	-0.048656	H	0.709634	8.102723	-0.079690
C	0.708864	4.844825	0.880801				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.250401 hartree
Thermal correction to Gibbs free energy = 0.202287 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8036.47903528 hartree

Reaction for 4n

Reactant1 of the reaction for 4n:

Atom	x	y	z	Atom	x	y	z
C	-2.054258	-2.542275	-1.728287	H	0.327627	6.392992	0.956235
C	-2.580612	-1.281857	-1.621882	C	3.368005	7.172131	2.262741
C	-1.804228	-0.230701	-1.070297	H	4.957595	5.744937	2.623672
C	-0.482601	-0.508828	-0.637223	N	-2.362625	1.009071	-0.961724
C	0.031854	-1.825966	-0.759993	S	-2.451397	3.588104	-0.412102
C	-0.729381	-2.836986	-1.295041	C	2.058761	7.343286	1.789600
C	0.267363	0.565621	-0.111406	C	-0.201251	-4.239760	-1.434441
C	-0.288092	1.826239	-0.028628	H	0.824015	-4.316524	-1.065774
C	-1.652618	1.986071	-0.461506	H	-0.821896	-4.946304	-0.873723
C	1.157148	3.854544	0.845288	H	-0.214506	-4.557684	-2.482053
C	0.484627	2.928364	0.444284	H	1.631520	8.340382	1.797949
H	-2.653857	-3.344315	-2.151183	O	3.987802	8.294074	2.696545
H	-3.590062	-1.054114	-1.948570	C	5.312037	8.168041	3.186213
H	1.046854	-2.023040	-0.423012	H	5.985378	7.790984	2.408961
H	1.292498	0.404774	0.210626	H	5.620294	9.170170	3.480757
C	1.910316	4.972067	1.321049	H	5.348742	7.502792	4.055623
C	3.217430	4.813019	1.794282	C	-2.445375	3.929245	1.377484
C	1.339882	6.258769	1.324993	H	-2.991569	4.865857	1.504903
C	3.947931	5.899924	2.263489	H	-1.429957	4.048340	1.756073
H	3.666908	3.825303	1.795463	H	-2.965445	3.136362	1.916381

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.319560 hartree
Thermal correction to Gibbs free energy = 0.266987 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -1300.33675680 hartree

Entrance1 of the reaction for 4n:

Atom	x	y	z	Atom	x	y	z
C	-2.322611	-3.029126	-0.152311	C	2.840879	4.385553	-0.309415
C	-1.052913	-2.848818	0.330230	C	2.316930	5.515006	-0.948439
C	-0.401011	-1.599852	0.167091	C	4.122237	4.460513	0.267773
C	-1.086738	-0.550654	-0.497651	C	3.045124	6.697134	-1.020343
C	-2.400597	-0.770818	-0.986953	H	1.327229	5.467214	-1.391544
C	-3.022049	-1.985525	-0.824368	C	4.851739	5.631413	0.198519
H	-2.817521	-3.988341	-0.024652	H	4.532220	3.590407	0.770807

H	-0.517075	-3.642005	0.841065	C	4.319150	6.758370	-0.445619
N	0.868961	-1.456562	0.643407	H	5.840414	5.705586	0.638122
C	-0.416151	0.685086	-0.623102	I	-0.674222	4.100887	1.043501
H	-2.912184	0.044117	-1.493216	I	-2.855714	5.372704	2.022321
C	0.857290	0.835847	-0.112950	C	-4.415318	-2.238952	-1.334420
C	1.475010	-0.306909	0.507855	H	-5.083049	-2.523814	-0.514851
H	-0.912437	1.525105	-1.101652	H	-4.827875	-1.352036	-1.820315
S	3.117572	-0.192315	1.209506	H	-4.420801	-3.061058	-2.057558
C	4.106510	0.152437	-0.281085	H	2.614178	7.555613	-1.520365
H	3.853485	1.120804	-0.714164	O	5.108772	7.854510	-0.458796
H	5.147560	0.166029	0.047330	C	4.611544	9.019977	-1.094532
H	3.974012	-0.642051	-1.016413	H	3.694220	9.371219	-0.610226
C	1.520467	2.098315	-0.174643	H	4.417480	8.836439	-2.156705
C	2.098912	3.166455	-0.239653	H	5.390415	9.773932	-0.991111

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.320444 hartree
Thermal correction to Gibbs free energy = 0.255418 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15081.3185891 hartree

TS1 of the reaction for 4n:

Atom	x	y	z	Atom	x	y	z
C	0.000000	0.000000	0.000000	H	4.599844	0.001084	1.554959
C	0.000000	0.000000	1.370204	H	3.144649	-2.243475	5.682244
C	1.227755	0.000000	2.078520	H	1.358256	-2.239458	5.805439
C	2.444170	0.000865	1.348923	H	2.357537	-1.934164	7.252546
C	2.408885	0.001680	-0.068968	C	5.843483	-1.346474	7.390052
C	1.213128	0.001055	-0.747067	C	5.671047	1.078945	7.629262
C	3.651525	0.000352	2.083911	C	6.362604	-1.444256	8.666360
N	1.198110	0.000080	3.442882	C	6.532554	-0.275042	9.429539
C	3.619655	-0.000612	3.457920	C	6.181623	0.985621	8.899689
C	2.327900	-0.003625	4.092998	H	5.713807	-2.239226	6.786884
C	4.812279	-0.006807	4.294751	H	5.395927	2.041913	7.212994
C	4.969993	-0.015303	5.556917	H	6.634265	-2.414405	9.061956
C	5.495114	-0.090463	6.847395	O	7.021012	-0.258288	10.670232
I	6.879784	-0.021005	3.327996	H	6.328984	1.862245	9.519914
I	9.494776	-0.053436	1.754551	H	0.617380	0.882236	-2.617436
S	2.252786	0.008209	5.881906	H	2.155879	0.003931	-2.687072
C	2.281151	-1.789923	6.173331	H	0.620898	-0.880653	-2.618405
H	-0.943319	-0.000120	-0.539637	C	7.402464	-1.491283	11.272779
H	-0.921462	-0.000027	1.942722	H	7.766357	-1.233535	12.265151
C	1.154723	0.001671	-2.250825	H	8.199957	-1.971223	10.698419
H	3.349175	0.002845	-0.614467	H	6.543163	-2.162993	11.355554

Number of imaginary frequencies = 1 (-119.5217 cm^{-1})
Zero-point vibrational correction = 0.320412 hartree

Thermal correction to Gibbs free energy = 0.259298 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15081.3096496 hartree

IM of the reaction for 4n:

Atom	x	y	z	Atom	x	y	z
C	-2.468697	-2.688322	-1.893874	C	1.373867	7.396273	1.745232
C	-2.795793	-1.393568	-1.589220	H	2.554526	6.300752	3.196067
C	-1.782821	-0.481714	-1.205573	N	-2.136089	0.808171	-0.914638
C	-0.428507	-0.927038	-1.140372	S	-1.437994	3.308314	-0.145204
C	-0.132435	-2.275573	-1.466037	I	3.099376	2.233078	0.169767
C	-1.123165	-3.152951	-1.837436	C	0.501282	7.283920	0.652542
C	0.578909	-0.009990	-0.750792	C	-0.822545	-4.585349	-2.184607
C	0.215065	1.278503	-0.441831	H	0.244644	-4.799491	-2.099065
C	-1.164957	1.578307	-0.559840	H	-1.365892	-5.265519	-1.520910
C	0.317120	3.546366	0.235848	H	-1.138871	-4.808642	-3.208530
C	1.017791	2.417113	-0.002008	H	0.112976	8.190963	0.202860
H	-3.248077	-3.385791	-2.188247	O	1.649815	8.652330	2.150036
H	-3.818643	-1.035441	-1.633103	C	2.541469	8.815832	3.241883
H	0.901703	-2.605632	-1.415356	H	3.523272	8.388572	3.013460
H	1.616669	-0.327314	-0.694759	H	2.635987	9.889917	3.392762
C	0.682329	4.870134	0.744214	H	2.140507	8.351511	4.148914
C	1.537490	4.993379	1.843952	C	-2.180104	3.174780	1.509810
C	0.159516	6.038522	0.161917	H	-3.197912	2.810223	1.366275
C	1.889663	6.241794	2.343526	H	-1.584576	2.489247	2.112100
H	1.927762	4.102315	2.323614	H	-2.187059	4.179974	1.933235
H	-0.501379	5.972251	-0.698235	I	6.519501	1.800380	0.419731

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.323141 hartree
Thermal correction to Gibbs free energy = 0.263936 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15081.3417947 hartree

Reactant2 of the reaction for 4n:

Atom	x	y	z	Atom	x	y	z
C	-2.472396	-2.692284	-1.882755	C	1.381393	7.394771	1.736829
C	-2.798321	-1.398509	-1.572746	H	2.527633	6.297571	3.214297
C	-1.782524	-0.487057	-1.197018	N	-2.133843	0.801654	-0.900213
C	-0.426524	-0.931442	-1.145597	S	-1.434997	3.303218	-0.135524
C	-0.132048	-2.278718	-1.476472	I	3.070752	2.269210	0.123651
C	-1.125923	-3.156028	-1.839963	C	0.524950	7.284316	0.630286
C	0.583366	-0.013880	-0.765054	C	-0.827981	-4.587425	-2.192136
C	0.218568	1.272548	-0.450750	H	0.240526	-4.800213	-2.121593
C	-1.162061	1.572750	-0.552714	H	-1.361480	-5.268193	-1.521192
C	0.317260	3.550517	0.229471	H	-1.158884	-4.810243	-3.211450
C	1.011756	2.419768	-0.020915	H	0.149439	8.192402	0.172201

H	-3.253772	-3.389915	-2.171059	O	1.659142	8.648500	2.139960
H	-3.821751	-1.041280	-1.606329	C	2.526199	8.813762	3.252105
H	0.902577	-2.608487	-1.436765	H	3.511058	8.381452	3.047798
H	1.621910	-0.330732	-0.720973	H	2.621419	9.888095	3.399389
C	0.688810	4.871461	0.735277	H	2.101393	8.355603	4.151142
C	1.527595	4.991525	1.848263	C	-2.159307	3.179375	1.528727
C	0.180673	6.040293	0.139972	H	-3.183131	2.828651	1.393754
C	1.879763	6.238918	2.348812	H	-1.567362	2.485943	2.125259
H	1.899550	4.099593	2.341273	H	-2.149015	4.185654	1.949672
H	-0.469445	5.974284	-0.728205				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.323093 hartree
Thermal correction to Gibbs free energy = 0.270490 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8190.67558889 hartree

Entrance2 of the reaction for 4n:

Atom	x	y	z	Atom	x	y	z
C	-2.469876	-2.691613	-1.889016	C	1.388918	7.391207	1.722471
C	-2.793689	-1.397328	-1.579655	H	2.508858	6.292968	3.218985
C	-1.776489	-0.485561	-1.207050	N	-2.127357	0.802996	-0.911039
C	-0.421321	-0.931313	-1.157383	S	-1.429155	3.301520	-0.140840
C	-0.128676	-2.279400	-1.488090	I	3.078056	2.268951	0.112780
C	-1.123610	-3.156237	-1.848736	C	0.546415	7.282119	0.605561
C	0.589301	-0.014274	-0.778132	C	-0.827580	-4.588751	-2.199031
C	0.225201	1.272113	-0.463688	H	0.241361	-4.801418	-2.133340
C	-1.155660	1.575865	-0.564090	H	-1.357117	-5.267963	-1.523329
C	0.322540	3.548882	0.213066	H	-1.163571	-4.814753	-3.216044
C	1.018287	2.418618	-0.034616	H	0.178587	8.190761	0.142300
H	-3.252712	-3.389246	-2.173486	O	1.667634	8.645762	2.126270
H	-3.817046	-1.039463	-1.609061	C	2.507613	8.807870	3.258842
H	0.905734	-2.610223	-1.448834	H	3.496226	8.372971	3.078625
H	1.627618	-0.331811	-0.733679	H	2.602499	9.881910	3.409279
C	0.698114	4.869142	0.718782	H	2.060148	8.350330	4.147094
C	1.523506	4.987853	1.841423	C	-2.149166	3.170932	1.542463
C	0.201808	6.038068	0.114919	H	-3.165990	2.800503	1.417426
C	1.874502	6.235167	2.343499	H	-1.542783	2.491358	2.138615
H	1.882541	4.095182	2.342657	H	-2.156801	4.176964	1.961208
H	-0.441173	5.971163	-0.758436	I	-3.606829	2.896501	4.655556

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.322979 hartree
Thermal correction to Gibbs free energy = 0.262698 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15081.3425438 hartree

TS2 of the reaction for 4n:

Atom	x	y	z	Atom	x	y	z
C	-2.483306	-2.652524	-1.960396	C	1.383530	7.404517	1.679846
C	-2.796671	-1.351375	-1.674260	H	2.396424	6.314675	3.255938
C	-1.782784	-0.450389	-1.258976	N	-2.128777	0.841007	-0.985590
C	-0.440304	-0.922227	-1.144612	S	-1.427322	3.321915	-0.188035
C	-0.157704	-2.280078	-1.451945	I	3.053746	2.239422	0.243477
C	-1.148238	-3.141792	-1.853399	C	0.600973	7.289642	0.521572
C	0.565602	-0.020956	-0.726300	C	-0.862431	-4.582122	-2.181409
C	0.210898	1.276665	-0.442257	H	0.196166	-4.816741	-2.051431
C	-1.160992	1.615746	-0.605160	H	-1.445030	-5.248671	-1.537356
C	0.300144	3.552687	0.192242	H	-1.140693	-4.806029	-3.216356
C	1.001651	2.410662	0.004431	H	0.279963	8.196041	0.020270
H	-3.264516	-3.337933	-2.277743	O	1.668623	8.663198	2.074080
H	-3.811191	-0.975948	-1.754593	C	2.446267	8.828558	3.248758
H	0.868016	-2.628398	-1.361344	H	3.432932	8.367313	3.134766
H	1.595072	-0.355929	-0.629487	H	2.558901	9.902932	3.384972
C	0.689424	4.875697	0.690748	H	1.938941	8.399257	4.119030
C	1.456631	5.001530	1.852447	C	-2.163392	3.079061	1.847383
C	0.253843	6.042105	0.039054	H	-3.144677	2.708497	1.584206
C	1.808198	6.252108	2.348965	H	-1.404972	2.374680	2.161316
H	1.769327	4.112092	2.389757	H	-2.061339	4.116236	2.136871
H	-0.345164	5.966901	-0.864232	I	-3.066901	2.756285	4.489003

Number of imaginary frequencies = 1 (-493.0980 cm^{-1})
Zero-point vibrational correction = 0.321745 hartree
Thermal correction to Gibbs free energy = 0.262519 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15081.3340140 hartree

Product of the reaction for 4n:

Atom	x	y	z	Atom	x	y	z
C	-2.464366	-2.667815	-1.958690	H	1.806284	4.117127	2.433800
C	-2.794420	-1.383518	-1.625029	H	-0.472627	5.911633	-0.733960
C	-1.792121	-0.471881	-1.192337	C	1.389287	7.396668	1.685950
C	-0.440853	-0.926396	-1.113884	H	2.483661	6.333522	3.224204
C	-0.140109	-2.271265	-1.470499	N	-2.161243	0.797014	-0.871657
C	-1.118162	-3.137403	-1.886349	S	-1.493513	3.266726	-0.017865
C	0.551389	-0.020970	-0.684025	I	3.022790	2.258874	0.267465
C	0.179184	1.263589	-0.354642	C	0.547392	7.261019	0.573894
C	-1.205485	1.595810	-0.478394	C	-0.811786	-4.561304	-2.266561
C	0.222666	3.515460	0.318459	H	0.253114	-4.780131	-2.160165
C	0.955443	2.393609	0.097472	H	-1.370780	-5.261449	-1.636992
H	-3.238301	-3.356154	-2.288401	H	-1.100574	-4.757987	-3.304349
H	-3.816874	-1.024275	-1.679478	H	0.202687	8.158301	0.071436
H	0.893611	-2.602973	-1.406118	O	1.698831	8.665079	2.041157
H	1.588948	-0.338378	-0.614574	C	2.546266	8.845870	3.162190

C	0.636786	4.847817	0.783139	H	3.522204	8.376172	2.998508
C	1.465301	4.996667	1.897691	H	2.673626	9.921758	3.273083
C	0.173432	6.003986	0.134389	H	2.091681	8.435471	4.070355
C	1.845839	6.256167	2.352329				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.283839 hartree
Thermal correction to Gibbs free energy = 0.233487 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8150.99496769 hartree

Reaction for 4o

Reactant1 of the reaction for 4o:

Atom	x	y	z	Atom	x	y	z
C	-1.829978	-4.155328	-1.980286	C	0.238353	4.204731	0.464517
C	-2.275264	-3.464132	-0.884147	C	0.589200	5.354783	0.639932
C	-1.798071	-2.153566	-0.628652	C	1.004509	6.707436	0.843610
C	-0.861163	-1.578769	-1.525650	C	0.497198	7.446600	1.923607
C	-0.419511	-2.321850	-2.651119	C	1.922494	7.301931	-0.036333
C	-0.887507	-3.591838	-2.888079	C	0.905667	8.760706	2.116347
C	-0.422444	-0.265694	-1.251034	H	-0.212420	6.982219	2.600348
C	-0.900434	0.405813	-0.143610	C	2.324240	8.616638	0.165601
C	-1.819986	-0.286889	0.721601	H	2.311123	6.725843	-0.869576
C	-0.156825	2.905716	0.266685	C	1.818058	9.347363	1.239972
C	-0.507888	1.754604	0.097708	H	0.511065	9.328848	2.952431
H	-2.198658	-5.159985	-2.170862	H	3.034002	9.072519	-0.517013
H	-2.991518	-3.891896	-0.190338	H	2.134453	10.373988	1.394166
H	0.298370	-1.865614	-3.328608	N	-2.247046	-1.497788	0.480458
C	-0.432946	-4.397166	-4.075698	S	-2.501438	0.518231	2.167492
H	0.284226	-3.840039	-4.682415	C	-0.994031	0.775500	3.157936
H	0.040722	-5.330276	-3.753761	H	-1.327879	1.203318	4.105024
H	-1.283449	-4.667350	-4.709957	H	-0.310484	1.471419	2.671222
H	0.276747	0.224903	-1.922336	H	-0.499895	-0.177491	3.350021

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.297726 hartree
Thermal correction to Gibbs free energy = 0.244701 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -1261.96693138 hartree

Entrance1 of the reaction for 4o:

Atom	x	y	z	Atom	x	y	z
C	0.004926	-0.009963	0.005601	H	4.599859	0.086177	1.589677
C	0.001049	-0.019652	1.375987	H	4.025163	-1.614815	6.020022

C	1.226019	-0.010326	2.089907	H	2.442029	-2.430405	5.808626
C	2.443230	0.012819	1.360676	H	2.887771	-1.729671	7.381456
C	2.412464	0.021737	-0.057997	C	8.068746	0.417510	6.169498
C	1.219224	0.010162	-0.739390	C	9.294282	0.523714	6.895808
C	3.643405	0.041453	2.102548	C	10.514210	0.615423	6.207353
N	1.188994	-0.038824	3.453601	C	9.282213	0.537016	8.299406
C	3.599184	0.037363	3.482166	C	11.703547	0.718629	6.918341
C	2.310811	-0.025350	4.121799	C	11.687686	0.731751	8.312809
C	4.804210	0.135509	4.237307	C	10.477592	0.641077	9.000186
C	5.850889	0.227767	4.853346	H	10.516243	0.605018	5.122584
C	7.026802	0.328370	5.551012	H	8.335958	0.466329	8.825146
I	4.506642	3.214291	5.205003	H	12.644899	0.789551	6.383605
I	3.942528	5.832673	5.575204	H	12.618794	0.813041	8.864178
S	2.181279	-0.018863	5.906043	H	10.465311	0.651670	10.085007
C	2.971156	-1.612859	6.299435	C	1.163735	0.018569	-2.243422
H	-0.937202	-0.018312	-0.536204	H	0.617278	0.894884	-2.606783
H	-0.922175	-0.037012	1.945436	H	2.165785	0.034630	-2.677586
H	3.354443	0.039776	-0.600487	H	0.641040	-0.867780	-2.617356

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298698 hartree
Thermal correction to Gibbs free energy = 0.233734 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15042.9467973 hartree

TS1 of the reaction for 4o:

Atom	x	y	z	Atom	x	y	z
C	0.000000	0.000000	0.000000	H	3.347894	-0.007368	-0.616652
C	0.000000	0.000000	1.370529	H	4.602028	-0.050706	1.551846
C	1.227169	0.000000	2.078613	H	1.559011	-2.231900	5.945822
C	2.444448	-0.003554	1.347043	H	0.223556	-1.089317	5.586282
C	2.407658	-0.004234	-0.071120	H	0.864856	-1.225126	7.251103
C	1.211930	-0.001662	-0.748810	C	5.861656	-0.469042	7.941856
C	3.652813	-0.022427	2.078897	C	6.402650	-0.581615	9.246407
N	1.199528	0.022623	3.442590	C	6.607076	-1.852440	9.814383
C	3.619715	-0.030287	3.453788	C	6.732592	0.579398	9.969429
C	2.329923	0.013092	4.086878	C	7.135993	-1.953765	11.092997
C	4.785545	-0.128968	4.308014	C	7.461193	-0.799442	11.807348
C	4.870022	-0.252767	5.579252	C	7.260040	0.463261	11.247357
C	5.407008	-0.367594	6.810967	H	6.349511	-2.738840	9.245036
I	6.877357	-0.115869	3.389247	H	6.571012	1.552370	9.518399
I	9.481750	-0.067065	1.854263	H	7.296444	-2.930995	11.534954
S	2.292925	0.076723	5.870408	H	7.874775	-0.884443	12.806958
C	1.113963	-1.267580	6.190716	H	7.516311	1.355070	11.808626
H	-0.943990	0.001955	-0.538497	H	0.620112	0.883356	-2.618725
H	-0.921728	0.004221	1.942530	H	2.152968	-0.004369	-2.689410
C	1.152110	-0.000615	-2.252508	H	0.612747	-0.879627	-2.619859

Number of imaginary frequencies = 1 (-183.6707 cm^{-1})
Zero-point vibrational correction = 0.297477 hartree
Thermal correction to Gibbs free energy = 0.236208 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15042.9318238 hartree

IM of the reaction for 4o:

Atom	x	y	z	Atom	x	y	z
C	-2.387793	-4.171349	-1.572164	C	0.070050	8.220073	2.588919
C	-2.716237	-3.094713	-0.790839	H	-1.153489	6.446527	2.653194
C	-1.962160	-1.901018	-0.883402	C	1.919466	8.172527	1.031362
C	-0.864339	-1.834995	-1.793573	H	2.135489	6.359058	-0.116944
C	-0.559105	-2.971582	-2.585453	C	1.174959	8.839069	2.004482
C	-1.297798	-4.126899	-2.487788	H	-0.508367	8.739868	3.345379
C	-0.110541	-0.638411	-1.874938	H	2.778470	8.654510	0.576804
C	-0.463623	0.418865	-1.070565	H	1.455891	9.842376	2.307673
C	-1.583190	0.212157	-0.224317	N	-2.316908	-0.837944	-0.095555
C	-0.471547	2.521314	0.005549	S	-1.906895	1.704557	0.739484
C	0.135738	1.735177	-0.917861	I	1.802049	2.354399	-2.010207
H	-2.968452	-5.086708	-1.498557	C	-0.984644	-5.339770	-3.320488
H	-3.546768	-3.124691	-0.093989	H	-0.127604	-5.163336	-3.973439
H	0.277518	-2.912371	-3.276412	H	-0.760729	-6.199345	-2.680768
H	0.732226	-0.563640	-2.557133	H	-1.843037	-5.612140	-3.942725
C	-0.172589	3.822101	0.438158	C	-1.290036	1.202477	2.375168
C	0.094905	4.943292	0.817955	H	-0.315883	0.728775	2.258553
C	0.452709	6.263375	1.226447	H	-1.228739	2.106618	2.981653
C	-0.295265	6.935790	2.204872	H	-2.029619	0.513048	2.784401
C	1.564656	6.888007	0.639168	I	4.562698	3.341685	-3.807092

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.300052 hartree
Thermal correction to Gibbs free energy = 0.239375 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15042.9685531 hartree

Reactant2 of the reaction for 4o:

Atom	x	y	z	Atom	x	y	z
C	-2.398719	-4.165881	-1.562587	C	0.018848	8.218795	2.561904
C	-2.719690	-3.082544	-0.787333	H	-1.205409	6.444365	2.563229
C	-1.956712	-1.895662	-0.887314	C	1.948650	8.170806	1.103665
C	-0.858545	-1.842714	-1.798959	H	2.226043	6.356878	-0.029761
C	-0.561565	-2.985652	-2.584343	C	1.152848	8.837326	2.035441
C	-1.308647	-4.135052	-2.478866	H	-0.598711	8.739281	3.286003
C	-0.096383	-0.652458	-1.887443	H	2.829898	8.653784	0.695295
C	-0.441598	0.409947	-1.086819	H	1.416665	9.841131	2.351815
C	-1.561129	0.217706	-0.238078	N	-2.301895	-0.825697	-0.105114

C	-0.437481	2.523895	-0.010038	S	-1.874959	1.715459	0.721532
C	0.156874	1.724658	-0.931275	I	1.797101	2.330020	-2.017987
H	-2.985644	-5.076635	-1.483225	C	-1.004902	-5.355504	-3.303360
H	-3.549989	-3.102599	-0.090012	H	-0.146479	-5.190614	-3.957409
H	0.274978	-2.937121	-3.276190	H	-0.788382	-6.212271	-2.657460
H	0.745175	-0.588788	-2.572199	H	-1.865744	-5.625025	-3.923326
C	-0.129532	3.821968	0.416629	C	-1.260727	1.217375	2.360099
C	0.134266	4.943124	0.800287	H	-0.296900	0.722822	2.245356
C	0.474536	6.262040	1.223547	H	-1.182706	2.125751	2.958232
C	-0.325118	6.934133	2.160830	H	-2.014204	0.546094	2.774334
C	1.615811	6.885953	0.694677				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.299912 hartree
Thermal correction to Gibbs free energy = 0.245253 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8152.30106865 hartree

Entrance2 of the reaction for 4o:

Atom	x	y	z	Atom	x	y	z
C	-2.398045	-4.163975	-1.578457	C	0.071071	8.183930	2.610924
C	-2.720611	-3.078977	-0.806586	H	-1.121738	6.388575	2.651941
C	-1.955229	-1.892844	-0.904021	C	1.912927	8.193997	1.042833
C	-0.852280	-1.843804	-1.809476	H	2.152844	6.404255	-0.136788
C	-0.553600	-2.988696	-2.592011	C	1.162467	8.830754	2.031300
C	-1.303186	-4.136273	-2.489234	H	-0.510346	8.680224	3.380559
C	-0.088065	-0.655012	-1.895539	H	2.762029	8.698176	0.593832
C	-0.436382	0.408739	-1.098354	H	1.429237	9.832669	2.351320
C	-1.560804	0.221649	-0.253409	N	-2.303786	-0.822097	-0.125337
C	-0.440249	2.523756	-0.028371	S	-1.877012	1.717766	0.701379
C	0.161197	1.723185	-0.943485	I	1.809141	2.324744	-2.022552
H	-2.986476	-5.073888	-1.499979	C	-0.996516	-5.358798	-3.309992
H	-3.553203	-3.096674	-0.111926	H	-0.136583	-5.194606	-3.962404
H	0.287456	-2.942932	-3.278685	H	-0.780005	-6.213615	-2.661443
H	0.757769	-0.593700	-2.575250	H	-1.855365	-5.631394	-3.931508
C	-0.129248	3.821960	0.397838	C	-1.266755	1.228415	2.363173
C	0.135530	4.941373	0.785206	H	-0.296730	0.746075	2.259858
C	0.477994	6.258867	1.212045	H	-1.204941	2.138493	2.958576
C	-0.275806	6.900965	2.206432	H	-2.012448	0.550006	2.776642
C	1.576753	6.911168	0.630225	I	-0.306976	0.292673	5.528043

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.299938 hartree
Thermal correction to Gibbs free energy = 0.238339 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15042.9676232 hartree

TS2 of the reaction for 4o:

Atom	x	y	z	Atom	x	y	z
C	-2.448792	-4.130848	-1.602717	C	-0.029717	8.255864	2.496768
C	-2.780936	-3.040339	-0.844797	H	-1.290476	6.507491	2.460804
C	-1.997963	-1.860632	-0.916374	C	1.962774	8.149644	1.130889
C	-0.865924	-1.830872	-1.786405	H	2.252213	6.316309	0.031978
C	-0.556394	-2.984228	-2.556032	C	1.140365	8.844481	2.017637
C	-1.322685	-4.120746	-2.477057	H	-0.668391	8.796794	3.186972
C	-0.086318	-0.653826	-1.849855	H	2.873236	8.607888	0.759404
C	-0.450025	0.419187	-1.069413	H	1.411998	9.845572	2.336268
C	-1.605576	0.258290	-0.253663	N	-2.358506	-0.790425	-0.148633
C	-0.493371	2.530474	-0.019082	S	-1.920632	1.732941	0.693190
C	0.149382	1.726122	-0.906832	I	1.837644	2.315301	-1.934783
H	-3.052388	-5.032379	-1.542690	C	-1.005715	-5.349892	-3.284681
H	-3.636827	-3.045547	-0.178527	H	-0.117886	-5.201383	-3.902863
H	0.308111	-2.950588	-3.214110	H	-0.829492	-6.208533	-2.628833
H	0.783395	-0.604826	-2.500109	H	-1.843360	-5.608556	-3.940423
C	-0.175946	3.833947	0.399510	C	-1.084771	1.082652	2.585556
C	0.093851	4.954615	0.778317	H	-0.147832	0.712899	2.191270
C	0.442959	6.272880	1.201252	H	-1.096473	2.046272	3.075658
C	-0.382725	6.974036	2.093234	H	-1.864456	0.372322	2.826065
C	1.620243	6.867485	0.720513	I	0.011438	0.225285	5.039908

Number of imaginary frequencies = 1 (-489.1614 cm^{-1})
Zero-point vibrational correction = 0.298576 hartree
Thermal correction to Gibbs free energy = 0.237567 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15042.9596550 hartree

Product of the reaction for 4o:

Atom	x	y	z	Atom	x	y	z
C	-2.338868	-4.162215	-1.646811	C	-0.207314	6.899543	2.203487
C	-2.638425	-3.108582	-0.828496	C	1.546949	6.904754	0.524924
C	-1.879095	-1.908077	-0.894501	C	0.139157	8.197249	2.560492
C	-0.802094	-1.829258	-1.829837	H	-1.018266	6.384442	2.707451
C	-0.524270	-2.949420	-2.663701	C	1.885066	8.202194	0.889506
C	-1.266441	-4.099387	-2.587336	H	2.085800	6.390746	-0.264372
C	-0.050323	-0.638934	-1.892699	C	1.183400	8.849998	1.906020
C	-0.384305	0.400086	-1.050647	H	-0.406922	8.700858	3.351332
C	-1.485041	0.197708	-0.159665	H	2.697506	8.709519	0.379798
C	-0.431148	2.462283	0.061995	H	1.450275	9.863329	2.188021
C	0.189611	1.708983	-0.889252	N	-2.210177	-0.883724	-0.063572
H	-2.925724	-5.075188	-1.587839	S	-1.774544	1.617740	0.837756
H	-3.453207	-3.154480	-0.113487	I	1.806494	2.373020	-1.995401
H	0.298181	-2.874324	-3.371147	C	-0.982802	-5.290485	-3.462730
H	0.775995	-0.546784	-2.593551	H	-0.141216	-5.099709	-4.132397
C	-0.116475	3.778137	0.460364	H	-0.746556	-6.171255	-2.856565

C	0.151917	4.909986	0.803421	H	-1.856795	-5.542154	-4.072433
C	0.496426	6.244553	1.181440				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.260778 hartree
Thermal correction to Gibbs free energy = 0.208908 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8112.62333600 hartree

Reaction for 4p

Reactant1 of the reaction for 4p:

Atom	x	y	z	Atom	x	y	z
C	-1.834459	-4.144970	-2.003895	C	0.241967	4.234826	0.469917
C	-2.263068	-3.434664	-0.906612	C	0.589269	5.385513	0.648353
C	-1.781271	-2.126567	-0.650436	C	1.000445	6.738886	0.855667
C	-0.845915	-1.541188	-1.542688	C	0.495237	7.471821	1.940918
C	-0.409639	-2.284418	-2.670935	C	1.912356	7.340386	-0.025833
C	-0.892303	-3.546746	-2.889790	C	0.899750	8.786601	2.137305
C	-0.407918	-0.230755	-1.262521	H	-0.209698	7.002113	2.618857
C	-0.885050	0.434626	-0.150402	C	2.310189	8.655707	0.179776
C	-1.801384	-0.266494	0.710937	H	2.299389	6.769167	-0.863202
C	-0.149134	2.935125	0.268520	C	1.806133	9.380192	1.259400
C	-0.496605	1.783331	0.096275	H	0.506770	9.349846	2.977498
C	-2.334348	-5.535081	-2.290039	H	3.015276	9.116944	-0.504066
H	-3.052746	-5.862319	-1.535513	H	2.119464	10.407309	1.416479
H	-2.819985	-5.577680	-3.270426	N	-2.228424	-1.476251	0.463784
H	-1.504237	-6.248832	-2.308635	S	-2.481576	0.527015	2.164167
H	-2.978385	-3.856526	-0.207030	C	-0.972031	0.792548	3.149051
H	0.306465	-1.834928	-3.353003	H	-1.305529	1.216107	4.098138
H	-0.557069	-4.112843	-3.754766	H	-0.294843	1.494025	2.661643
H	0.289325	0.264056	-1.932793	H	-0.470890	-0.157362	3.337598

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.297704 hartree
Thermal correction to Gibbs free energy = 0.244719 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -1261.9675284 hartree

Entrance1 of the reaction for 4p:

Atom	x	y	z	Atom	x	y	z
C	-0.021974	-0.000014	-0.003484	H	4.608407	0.083130	1.581103
C	0.004059	-0.012550	1.371721	H	4.040373	-1.604814	6.019546
C	1.231941	-0.007213	2.078336	H	2.464089	-2.431193	5.799154
C	2.452563	0.014246	1.354091	H	2.895669	-1.727112	7.374234

C	2.413493	0.026429	-0.065164	C	8.070981	0.415651	6.171844
C	1.210305	0.019163	-0.718547	C	9.294279	0.522400	6.901907
C	3.652021	0.039280	2.094262	C	10.515219	0.627488	6.217142
N	1.196128	-0.037757	3.443200	C	9.279040	0.522806	8.305544
C	3.607918	0.033619	3.474407	C	11.702354	0.731047	6.931771
C	2.318185	-0.027527	4.111002	C	11.683341	0.731260	8.326267
C	4.811750	0.131836	4.230665	C	10.472226	0.627332	9.009994
C	5.857120	0.225092	4.848986	H	10.519774	0.627057	5.132322
C	7.031064	0.326018	5.549958	H	8.332051	0.441856	8.828492
I	4.520446	3.214052	5.181637	H	12.644470	0.812302	6.399825
I	3.958817	5.835098	5.537545	H	12.612724	0.812836	8.880496
S	2.185373	-0.021740	5.895272	H	10.457442	0.627915	10.094846
C	2.984830	-1.609929	6.292704	C	-1.317325	-0.006646	-0.769100
H	-0.913305	-0.029225	1.952460	H	-2.176884	-0.021339	-0.095762
H	1.183512	0.028934	-1.804765	H	-1.393910	0.879694	-1.407286
H	3.348103	0.043658	-0.618118	H	-1.375836	-0.882869	-1.423031

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298674 hartree
Thermal correction to Gibbs free energy = 0.233635 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15042.9471549 hartree

TS1 of the reaction for 4p:

Atom	x	y	z	Atom	x	y	z
C	0.000000	0.000000	0.000000	H	3.381077	-0.007738	-0.552673
C	0.000000	0.000000	1.375733	H	4.602605	-0.050991	1.650884
C	1.214681	0.000000	2.102740	H	1.434744	-2.220190	5.980724
C	2.450873	-0.003581	1.402437	H	0.124198	-1.060046	5.587282
C	2.436399	-0.004456	-0.017056	H	0.724424	-1.200369	7.267234
C	1.245250	-0.002085	-0.692242	C	5.717909	-0.480179	8.069374
C	3.642495	-0.022638	2.157908	C	6.230489	-0.596948	9.384945
N	1.159173	0.022573	3.467056	C	6.424653	-1.869708	9.952249
C	3.579927	-0.030799	3.532392	C	6.542832	0.561676	10.119543
C	2.276011	0.012848	4.134473	C	6.926090	-1.975313	11.241539
C	4.725331	-0.131171	4.412777	C	7.233824	-0.823328	11.967304
C	4.778449	-0.257988	5.686107	C	7.042693	0.441294	11.408126
C	5.288102	-0.375719	6.928996	H	6.180933	-2.754199	9.373914
I	6.835272	-0.116523	3.543587	H	6.389471	1.536166	9.668924
I	9.481255	-0.066976	2.074030	H	7.078651	-2.954034	11.682985
S	2.201838	0.077784	5.916867	H	7.625855	-0.911699	12.975277
C	0.997397	-1.249295	6.213067	H	7.285263	1.331233	11.978370
C	-1.280773	0.003142	-0.789250	H	-2.153082	0.002849	-0.132434
H	-0.928166	0.004604	1.939137	H	-1.334340	0.885942	-1.434591
H	1.238541	-0.001848	-1.778674	H	-1.336458	-0.876638	-1.438526

Number of imaginary frequencies = 1 (-182.0773 cm^{-1})

Zero-point vibrational correction = 0.297420 hartree
Thermal correction to Gibbs free energy = 0.235825 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15042.9322456 hartree

IM of the reaction for 4p:

Atom	x	y	z	Atom	x	y	z
C	-2.404970	-4.197913	-1.548288	H	-1.166276	6.446374	2.651126
C	-2.712518	-3.101342	-0.776364	C	1.894899	8.182028	1.017487
C	-1.956751	-1.911056	-0.876268	H	2.116056	6.366803	-0.127043
C	-0.858854	-1.837846	-1.786239	C	1.149860	8.847675	1.990839
C	-0.558663	-2.979869	-2.574754	H	-0.529657	8.744149	3.336153
C	-1.309457	-4.118429	-2.455127	H	2.750627	8.666694	0.559619
C	-0.107636	-0.642351	-1.870600	H	1.427070	9.852959	2.290876
C	-0.461950	0.416096	-1.066733	N	-2.311862	-0.845706	-0.088751
C	-1.580042	0.205102	-0.220598	S	-1.907312	1.698195	0.743296
C	-0.475098	2.518897	0.008637	I	1.797005	2.356698	-2.009372
C	0.133557	1.733575	-0.914869	H	-1.071797	-4.987305	-3.062348
H	-3.540363	-3.119795	-0.074418	C	-3.196046	-5.473465	-1.458227
H	0.274007	-2.932234	-3.269698	H	-3.633874	-5.723787	-2.429814
H	0.734144	-0.567419	-2.554043	H	-2.549110	-6.307942	-1.169240
C	-0.179984	3.821349	0.438925	H	-4.002159	-5.391205	-0.726582
C	0.083926	4.944312	0.815967	C	-1.288669	1.194821	2.378016
C	0.437050	6.266849	1.220738	H	-0.312477	0.725561	2.260440
C	-0.311369	6.938311	2.199412	H	-1.231331	2.097811	2.986550
C	1.544795	6.895025	0.629250	H	-2.025473	0.501234	2.785265
C	0.049212	8.225162	2.579486	I	4.552559	3.350537	-3.811513

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.300059 hartree
Thermal correction to Gibbs free energy = 0.239384 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15042.9689491 hartree

Reactant2 of the reaction for 4p:

Atom	x	y	z	Atom	x	y	z
C	-2.416092	-4.195613	-1.536276	H	-1.225316	6.443851	2.550930
C	-2.715231	-3.092093	-0.770427	C	1.924323	8.178342	1.091631
C	-1.950565	-1.909012	-0.878465	H	2.211941	6.361440	-0.034414
C	-0.852593	-1.849134	-1.790409	C	1.123698	8.845005	2.019171
C	-0.561463	-2.997731	-2.572511	H	-0.630105	8.744043	3.266359
C	-1.320796	-4.129659	-2.444689	H	2.804333	8.663582	0.683256
C	-0.092828	-0.660328	-1.882505	H	1.382476	9.851172	2.332189
C	-0.438850	0.403709	-1.082672	N	-2.295740	-0.836264	-0.096918
C	-1.556846	0.207666	-0.233691	S	-1.873953	1.706691	0.725145
C	-0.439691	2.518647	-0.007944	I	1.793548	2.328023	-2.017834
C	0.155858	1.719616	-0.928852	H	-1.090422	-5.004076	-3.046634

H	-3.542275	-3.100213	-0.067501	C	-3.215847	-5.464615	-1.437597
H	0.270655	-2.961182	-3.268763	H	-3.653984	-5.718681	-2.407986
H	0.747498	-0.596969	-2.568850	H	-2.574308	-6.300964	-1.142210
C	-0.135796	3.818633	0.415966	H	-4.021897	-5.371560	-0.707378
C	0.123845	4.941889	0.796282	C	-1.257459	1.208744	2.362924
C	0.458214	6.263649	1.215546	H	-0.291866	0.717825	2.247295
C	-0.346237	6.935869	2.148603	H	-1.182374	2.116737	2.961974
C	1.597903	6.890532	0.686789	H	-2.008396	0.534281	2.776622
C	-0.008697	8.223536	2.545568				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.299900 hartree
Thermal correction to Gibbs free energy = 0.245059 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8152.30155432 hartree

Entrance2 of the reaction for 4p:

Atom	x	y	z	Atom	x	y	z
C	-2.411566	-4.195250	-1.548735	H	-1.136151	6.387091	2.646400
C	-2.714094	-3.089596	-0.787991	C	1.886604	8.202365	1.026177
C	-1.947981	-1.906592	-0.894215	H	2.132293	6.410734	-0.149363
C	-0.844852	-1.850647	-1.799579	C	1.135333	8.838253	2.014576
C	-0.550517	-3.001585	-2.577406	H	-0.533908	8.683406	3.367749
C	-1.311391	-4.132509	-2.451574	H	2.732383	8.709291	0.573999
C	-0.083798	-0.662679	-1.889815	H	1.398094	9.842247	2.331386
C	-0.433924	0.402869	-1.094251	N	-2.297601	-0.832834	-0.117168
C	-1.557032	0.211856	-0.249270	S	-1.877456	1.709276	0.704085
C	-0.443859	2.519189	-0.026955	I	1.804754	2.323822	-2.022507
C	0.159307	1.718838	-0.941370	H	-1.077858	-5.008915	-3.049506
H	-3.543753	-3.095542	-0.088132	C	-3.211526	-5.464375	-1.449373
H	0.286353	-2.967503	-3.268170	H	-3.644365	-5.723463	-2.420919
H	0.761074	-0.601489	-2.570783	H	-2.571504	-6.299030	-1.145917
C	-0.137219	3.819404	0.396371	H	-4.021490	-5.368453	-0.723795
C	0.123593	4.940845	0.780536	C	-1.265590	1.220507	2.365532
C	0.461052	6.260964	1.203421	H	-0.293684	0.742026	2.261876
C	-0.293538	6.902205	2.197750	H	-1.207279	2.130193	2.961841
C	1.555502	6.916909	0.617614	H	-2.008773	0.538766	2.778060
C	0.048215	8.187834	2.598176	I	-0.304660	0.284458	5.529774

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.299938 hartree
Thermal correction to Gibbs free energy = 0.238331 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15042.9681100 hartree

TS2 of the reaction for 4p:

Atom	x	y	z	Atom	x	y	z

C	-2.449979	-4.170069	-1.558754	H	-1.314242	6.510198	2.446811
C	-2.761384	-3.060907	-0.809520	C	1.928864	8.162624	1.105078
C	-1.978836	-1.883025	-0.889772	H	2.230561	6.322524	0.020880
C	-0.847955	-1.844631	-1.761629	C	1.101651	8.859242	1.985932
C	-0.542622	-3.002611	-2.527874	H	-0.707273	8.809162	3.154896
C	-1.319503	-4.123678	-2.426537	H	2.836464	8.623766	0.730175
C	-0.073415	-0.666800	-1.830690	H	1.366602	9.864641	2.296527
C	-0.439579	0.407233	-1.051579	N	-2.340504	-0.810865	-0.122921
C	-1.592004	0.240468	-0.233319	S	-1.912554	1.715874	0.711520
C	-0.492446	2.520892	-0.006679	I	1.834233	2.313763	-1.928700
C	0.152557	1.717521	-0.893829	H	-1.077990	-5.004055	-3.015546
H	-3.613565	-3.056259	-0.136915	C	-3.270133	-5.428622	-1.485881
H	0.316667	-2.978760	-3.191388	H	-3.675793	-5.682095	-2.470695
H	0.793998	-0.616285	-2.483941	H	-2.652661	-6.272860	-1.162441
C	-0.182734	3.828257	0.405486	H	-4.101856	-5.321580	-0.786716
C	0.080381	4.953050	0.776691	C	-1.067191	1.069542	2.600672
C	0.421189	6.276614	1.189861	H	-0.126960	0.710726	2.204119
C	-0.409297	6.979575	2.075935	H	-1.088163	2.031470	3.093739
C	1.594788	6.875026	0.704844	H	-1.838938	0.350351	2.840611
C	-0.064761	8.266859	2.469338	I	0.043566	0.216606	5.050740

Number of imaginary frequencies = 1 (-488.9564 cm^{-1})
Zero-point vibrational correction = 0.298605 hartree
Thermal correction to Gibbs free energy = 0.237771 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15042.9601890 hartree

Product of the reaction for 4p:

Atom	x	y	z	Atom	x	y	z
C	-2.358673	-4.183220	-1.635459	C	1.556143	6.897777	0.536108
C	-2.646433	-3.105681	-0.836399	C	0.112568	8.209432	2.533931
C	-1.877362	-1.912264	-0.900221	H	-1.056094	6.402844	2.668141
C	-0.782908	-1.837067	-1.816113	C	1.892674	8.195962	0.899516
C	-0.501281	-2.966727	-2.636607	H	2.108859	6.376333	-0.238609
C	-1.263120	-4.097232	-2.547346	C	1.173152	8.853349	1.897239
C	-0.025551	-0.651656	-1.873491	H	-0.447428	8.720484	3.310147
C	-0.369745	0.393380	-1.042455	H	2.717892	8.696335	0.403636
C	-1.485938	0.197153	-0.169931	H	1.438800	9.867237	2.178412
C	-0.429727	2.461005	0.059045	N	-2.217170	-0.881061	-0.080120
C	0.204673	1.701381	-0.877974	S	-1.788028	1.622360	0.815900
H	-3.471768	-3.133407	-0.131083	I	1.839853	2.356696	-1.962407
H	0.330374	-2.909928	-3.333207	H	-1.040080	-4.953725	-3.177791
H	0.812614	-0.566958	-2.561137	C	-3.166873	-5.451136	-1.576070
C	-0.118891	3.778071	0.456177	H	-3.615948	-5.670229	-2.550459
C	0.146731	4.910981	0.797944	H	-2.531710	-6.303722	-1.313892
C	0.489182	6.246434	1.174734	H	-3.967463	-5.378156	-0.836864
C	-0.232480	6.911066	2.177907				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.260789 hartree
Thermal correction to Gibbs free energy = 0.209133 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8112.62383694 hartree

Reaction for 4q

Reactant1 of the reaction for 4q:

Atom	x	y	z	Atom	x	y	z
C	-1.788607	-4.125323	-2.058638	C	0.995171	6.734813	0.864810
C	-2.232836	-3.438888	-0.955748	C	0.480722	7.457675	1.952453
C	-1.755266	-2.130795	-0.694648	C	1.909246	7.346395	-0.007458
C	-0.819160	-1.542063	-1.585378	C	0.878288	8.772811	2.160249
C	-0.375640	-2.273398	-2.717307	H	-0.225830	6.980055	2.623169
C	-0.852035	-3.539276	-2.946936	C	2.300073	8.661984	0.209572
C	-0.384733	-0.229348	-1.298890	H	2.303395	6.782778	-0.846618
C	-0.864241	0.430034	-0.185940	C	1.786795	9.376536	1.291436
C	-1.781023	-0.275786	0.673712	H	0.478197	9.328407	3.002140
C	-0.136618	2.930729	0.246699	H	3.006846	9.131188	-0.467096
C	-0.479442	1.778807	0.066944	H	2.094606	10.403933	1.457408
H	-2.154787	-5.127552	-2.256567	N	-2.204839	-1.484648	0.421725
H	-2.947441	-3.868778	-0.261727	S	-2.464445	0.511846	2.128190
H	0.340141	-1.813808	-3.392804	C	-0.956618	0.778589	3.115523
H	-0.513801	-4.099279	-3.812507	H	-1.293631	1.190849	4.068371
H	0.311897	0.269386	-1.966816	H	-0.284064	1.489143	2.634976
C	0.248941	4.230514	0.457722	H	-0.449325	-0.169819	3.295501
C	0.590872	5.381261	0.645681				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.269959 hartree
Thermal correction to Gibbs free energy = 0.219218 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -1222.65909008 hartree

Entrance1 of the reaction for 4q:

Atom	x	y	z	Atom	x	y	z
C	0.000000	0.000000	0.000000	H	1.195596	0.005834	-1.808859
C	0.000000	0.000000	1.373200	H	3.359236	0.018021	-0.606343
C	1.226590	0.000000	2.082083	H	4.604723	0.068546	1.589009
C	2.447870	0.008745	1.356869	H	4.024449	-1.603745	6.023771
C	2.419797	0.010720	-0.061552	H	2.444583	-2.423323	5.803045
C	1.218585	0.005145	-0.724303	H	2.879298	-1.721629	7.378367
C	3.647497	0.031778	2.101063	C	8.068110	0.414061	6.170713

N	1.189065	-0.024891	3.447441	C	9.293699	0.522006	6.896586
C	3.601019	0.033379	3.479678	C	10.510829	0.642512	6.207582
C	2.309347	-0.019816	4.116484	C	9.284460	0.508286	8.300189
C	4.804658	0.130903	4.236981	C	11.700298	0.747366	6.918131
C	5.850847	0.222914	4.853867	C	11.687285	0.733531	8.312602
C	7.026340	0.323803	5.552009	C	10.479924	0.614211	9.000520
I	4.508748	3.213663	5.202675	H	10.510612	0.652930	5.122832
I	3.946353	5.832207	5.572721	H	8.340338	0.415464	8.826316
S	2.176112	-0.012700	5.900369	H	12.639542	0.840593	6.383011
C	2.968907	-1.604537	6.296872	H	12.618511	0.816167	8.863645
H	-0.940494	-0.002992	-0.541206	H	10.469915	0.603897	10.085325
H	-0.920386	-0.005646	1.947162				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.270961 hartree
Thermal correction to Gibbs free energy = 0.208277 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15003.6388459 hartree

TS1 of the reaction for 4q:

Atom	x	y	z	Atom	x	y	z
C	0.000000	0.000000	0.000000	H	1.195417	-0.001751	-1.808678
C	0.000000	0.000000	1.373242	H	3.359143	-0.008120	-0.606897
C	1.226649	0.000000	2.080008	H	4.607140	-0.051680	1.571162
C	2.450116	-0.003736	1.356291	H	1.521211	-2.221430	5.950099
C	2.420042	-0.004690	-0.061760	H	0.197966	-1.064889	5.589594
C	1.218378	-0.002103	-0.724213	H	0.836133	-1.207939	7.255212
C	3.655655	-0.022817	2.094116	C	5.826805	-0.477081	7.969342
N	1.194328	0.023060	3.445517	C	6.360782	-0.592236	9.276513
C	3.615799	-0.030464	3.467910	C	6.559921	-1.864139	9.843966
C	2.321384	0.013711	4.093671	C	6.689026	0.567348	10.002603
C	4.776028	-0.130602	4.329452	C	7.081934	-1.967926	11.125207
C	4.847679	-0.256030	5.601842	C	7.405488	-0.815032	11.842614
C	5.378463	-0.373387	6.836154	C	7.209587	0.448715	11.283113
I	6.872558	-0.118127	3.424929	H	6.303767	-2.749384	9.272195
I	9.489947	-0.070746	1.910460	H	6.531570	1.541141	9.551894
S	2.278732	0.079417	5.876836	H	7.238310	-2.945958	11.566838
C	1.085638	-1.252860	6.195057	H	7.813665	-0.901992	12.844274
H	-0.940577	0.002136	-0.540868	H	7.464552	1.339374	11.846790
H	-0.920431	0.004545	1.947099				

Number of imaginary frequencies = 1 (-183.1871 cm^{-1})
Zero-point vibrational correction = 0.269745 hartree
Thermal correction to Gibbs free energy = 0.210662 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15003.6238798 hartree

IM of the reaction for 4q:

Atom	x	y	z	Atom	x	y	z
C	-2.463930	-4.158350	-1.575533	C	-0.336963	6.951278	2.158517
C	-2.794845	-3.063658	-0.815583	C	1.596497	6.862822	0.686392
C	-2.014943	-1.887468	-0.900093	C	0.030930	8.231497	2.553492
C	-0.886583	-1.844364	-1.775100	H	-1.224272	6.479031	2.566651
C	-0.574593	-2.993489	-2.546218	C	1.953597	8.143423	1.089174
C	-1.346991	-4.123104	-2.446465	H	2.194599	6.319929	-0.038060
C	-0.111905	-0.659870	-1.844384	C	1.173726	8.828162	2.021076
C	-0.473836	0.410493	-1.062764	H	-0.574967	8.765325	3.277963
C	-1.623352	0.227622	-0.250266	H	2.842063	8.608123	0.675093
C	-0.486645	2.524258	-0.009809	H	1.456701	9.828293	2.332748
C	0.138922	1.719842	-0.904720	N	-2.376960	-0.808392	-0.134018
H	-3.061682	-5.061273	-1.512143	S	-1.958243	1.737548	0.684248
H	-3.646026	-3.066601	-0.143632	I	1.847441	2.303706	-1.950878
H	0.282630	-2.959805	-3.211355	C	-1.410338	1.250254	2.348700
H	-1.104225	-4.999199	-3.037929	H	-0.436336	0.767543	2.277776
H	0.752864	-0.605535	-2.500474	H	-1.365663	2.161429	2.946097
C	-0.183073	3.824498	0.420823	H	-2.171390	0.572048	2.736711
C	0.086308	4.944101	0.804034	I	4.678573	3.227300	-3.662287
C	0.446541	6.260638	1.221502				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.272167 hartree
Thermal correction to Gibbs free energy = 0.212797 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15003.6601239 hartree

Reactant2 of the reaction for 4q:

Atom	x	y	z	Atom	x	y	z
C	-2.479147	-4.159635	-1.551319	C	-0.346163	6.929098	2.130216
C	-2.799461	-3.056228	-0.799251	C	1.632573	6.870174	0.715600
C	-2.009976	-1.887949	-0.896017	C	-0.001709	8.208717	2.546556
C	-0.883020	-1.861519	-1.774491	H	-1.240989	6.445126	2.506866
C	-0.582523	-3.019040	-2.537242	C	1.965601	8.150138	1.139479
C	-1.364504	-4.140909	-2.425713	H	2.257201	6.338997	0.005120
C	-0.098800	-0.684669	-1.855471	C	1.151295	8.819391	2.053205
C	-0.450611	0.393497	-1.080490	H	-0.633536	8.731228	3.256780
C	-1.599557	0.229317	-0.264007	H	2.861557	8.627177	0.756941
C	-0.450125	2.523720	-0.037131	H	1.415651	9.819233	2.381461
C	0.162754	1.701228	-0.924895	N	-2.360976	-0.798809	-0.139606
H	-3.083941	-5.057073	-1.479001	S	-1.929140	1.752742	0.651049
H	-3.648688	-3.046751	-0.125067	I	1.847706	2.264054	-1.964630
H	0.272831	-2.998666	-3.205283	C	-1.401554	1.295843	2.330689
H	-1.131252	-5.023890	-3.010605	H	-0.430840	0.804268	2.282296
H	0.763438	-0.644210	-2.515779	H	-1.360411	2.219449	2.909284
C	-0.134619	3.820757	0.386479	H	-2.173343	0.630975	2.720793

C	0.131197	4.939600	0.775623	C	-2.479147	-4.159635	-1.551319
C	0.472272	6.254177	1.211204				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.272087 hartree
Thermal correction to Gibbs free energy = 0.219550 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8112.99254660 hartree

Entrance2 of the reaction for 4q:

Atom	x	y	z	Atom	x	y	z
C	-2.472328	-4.151900	-1.586634	C	-0.329576	6.925740	2.133481
C	-2.796551	-3.049275	-0.835552	C	1.610904	6.884969	0.667247
C	-2.007822	-1.879527	-0.927560	C	0.017920	8.206026	2.545668
C	-0.877593	-1.851823	-1.801207	H	-1.209514	6.433738	2.533821
C	-0.572779	-3.008903	-2.563398	C	1.947399	8.165352	1.087194
C	-1.353751	-4.131659	-2.456239	H	2.220595	6.359558	-0.060311
C	-0.094628	-0.674058	-1.877715	C	1.153416	8.826152	2.024561
C	-0.450710	0.402225	-1.102341	H	-0.597399	8.720935	3.275681
C	-1.601858	0.237452	-0.287634	H	2.830799	8.648799	0.683915
C	-0.458163	2.528105	-0.054731	H	1.420667	9.826042	2.350468
C	0.159025	1.710519	-0.943849	N	-2.362430	-0.793357	-0.169628
H	-3.075933	-5.050350	-1.516262	S	-1.926578	1.749184	0.641184
H	-3.647256	-3.041266	-0.163182	I	1.843893	2.279777	-1.982247
H	0.286356	-2.987391	-3.226649	C	-1.373462	1.271122	2.326454
H	-1.116188	-5.014488	-3.039748	H	-0.402806	0.783946	2.260168
H	0.770790	-0.632007	-2.533806	H	-1.327205	2.186163	2.915764
C	-0.142393	3.825799	0.368986	H	-2.135608	0.599325	2.720307
C	0.124260	4.944357	0.757639	I	-0.460726	0.343398	5.505255
C	0.467923	6.259533	1.190298				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.272117 hartree
Thermal correction to Gibbs free energy = 0.211938 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15003.6592498 hartree

TS2 of the reaction for 4q:

Atom	x	y	z	Atom	x	y	z
C	-2.516535	-4.101455	-1.625402	C	-0.316828	6.957893	2.134230
C	-2.854296	-2.991217	-0.894026	C	1.582824	6.911620	0.618570
C	-2.040837	-1.832763	-0.947404	C	0.032404	8.245718	2.521617
C	-0.869167	-1.832299	-1.765687	H	-1.183008	6.465693	2.563489
C	-0.550655	-2.999169	-2.510602	C	1.921763	8.199678	1.013141
C	-1.356054	-4.105987	-2.440991	H	2.176209	6.381513	-0.119109
C	-0.060726	-0.672954	-1.802950	C	1.149002	8.867442	1.963111
C	-0.435844	0.414697	-1.050004	H	-0.567355	8.765554	3.261182

C	-1.633294	0.286126	-0.289654	H	2.790347	8.683909	0.579509
C	-0.479406	2.533321	-0.014427	H	1.417477	9.873357	2.268950
C	0.185672	1.708405	-0.866433	N	-2.412055	-0.744286	-0.207662
H	-3.140479	-4.987876	-1.582543	S	-1.960687	1.776524	0.628587
H	-3.736575	-2.965408	-0.263824	I	1.934484	2.249388	-1.816017
H	0.340144	-2.994880	-3.131441	C	-1.289543	1.080998	2.567188
H	-1.107928	-4.994830	-3.010995	H	-0.317901	0.722730	2.254023
H	0.839433	-0.650404	-2.411882	H	-1.350530	2.027547	3.085718
C	-0.157441	3.836860	0.400445	H	-2.086378	0.363190	2.709641
C	0.112260	4.960646	0.769837	I	-0.456753	0.128968	5.092518
C	0.458947	6.283966	1.178697				

Number of imaginary frequencies = 1 (-490.8288 cm^{-1})
Zero-point vibrational correction = 0.270854 hartree
Thermal correction to Gibbs free energy = 0.211871 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -15003.6514934 hartree

Product of the reaction for 4q:

Atom	x	y	z	Atom	x	y	z
C	-2.398272	-4.144460	-1.683050	C	-0.124546	3.777599	0.453672
C	-2.704903	-3.077044	-0.881159	C	0.147057	4.907726	0.799842
C	-1.921274	-1.892638	-0.930874	C	0.497094	6.239354	1.182894
C	-0.810181	-1.832032	-1.828791	C	-0.238086	6.913210	2.169966
C	-0.520898	-2.960100	-2.647041	C	1.585375	6.877212	0.567019
C	-1.294700	-4.087041	-2.576081	C	0.114839	8.207564	2.532733
C	-0.038775	-0.652503	-1.871920	H	-1.078137	6.415223	2.642498
C	-0.385839	0.395139	-1.047632	C	1.929588	8.171498	0.937007
C	-1.519658	0.211942	-0.192986	H	2.148331	6.348524	-0.195310
C	-0.442330	2.463572	0.052175	C	1.196636	8.838129	1.918713
C	0.199736	1.697434	-0.874080	H	-0.455511	8.725923	3.296450
H	-3.001425	-5.045508	-1.639671	H	2.771307	8.661575	0.458908
H	-3.543102	-3.099916	-0.192744	H	1.468392	9.848919	2.205141
H	0.324860	-2.905997	-3.326529	N	-2.263567	-0.857244	-0.116135
H	-1.069078	-4.943520	-3.202579	S	-1.822131	1.640685	0.787542
H	0.812034	-0.576894	-2.544881	I	1.856664	2.336453	-1.934409

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.233010 hartree
Thermal correction to Gibbs free energy = 0.183537 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -8703.31566344 hartree

DFT-optimized cartesian coordinates [Å] and energies [hartree] of all the stationary points in the reactions of X = Se.

Reaction for 7a

Reactant1 of the reaction for 7a:

Atom	x	y	z	Atom	x	y	z
C	-2.217468	-2.671834	-1.210177	H	1.547304	0.351641	-1.739367
C	-2.460067	-1.525085	-0.501153	H	2.747557	4.389056	-1.776794
C	-1.503634	-0.477802	-0.494156	N	-1.768084	0.646603	-0.572097
C	-0.302966	-0.641293	-1.231590	Se	-1.352302	3.185282	0.232935
C	-0.082234	-1.842050	-1.954766	C	-0.800463	-4.132021	1.241274
C	-1.015213	-2.850730	-1.953568	H	-0.821751	-4.992886	-2.713761
C	0.621243	0.426793	-1.213598	H	-1.592870	-4.281905	-2.037590
C	0.339784	1.569999	-0.497250	H	0.159602	-4.128495	-3.454261
C	-0.894176	1.616785	0.236021	H	-2.953651	-3.471605	-3.234458
C	2.050566	3.579353	-0.543902	C	0.036196	3.040233	-1.211921
C	1.252433	2.674382	-0.509092	H	-0.112922	3.886145	2.605310
H	-3.373872	-1.386358	0.067277	H	1.022445	3.100521	3.276860
H	0.843332	-1.950886	-2.515201	H	-0.095560	2.107299	2.147013

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.202286 hartree
Thermal correction to Gibbs free energy = 0.160200 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -2958.16165338 hartree

Entrance1 of the reaction for 7a:

Atom	x	y	z	Atom	x	y	z
C	0.914479	-0.034655	-0.508965	H	3.398778	2.233512	0.047238
C	0.783272	-0.569667	0.745949	H	4.051409	2.176700	2.439769
C	1.603791	-0.102511	1.804055	H	4.435220	-1.017225	6.159146
C	2.546863	0.920579	1.536710	H	3.973851	-2.436949	5.160727
C	2.662386	1.453056	0.226264	H	3.636318	-2.425523	6.909763
C	1.863164	0.990421	-0.791744	N	7.046221	4.320084	2.117404
C	3.334604	1.380357	2.614229	C	6.414536	4.241684	0.879105
N	1.469783	-0.664347	3.040346	C	8.211567	5.088247	2.115260
C	3.177865	0.827627	3.868511	C	7.234326	5.052773	-0.107935
C	2.220026	-0.234853	4.019501	O	5.395380	3.626608	0.668408
C	3.926200	1.321627	4.988812	C	8.412714	5.605619	0.701046
C	4.547677	1.744546	5.937263	O	8.903669	5.280090	3.083492
H	5.066296	2.098762	6.803380	H	6.595181	5.831735	-0.529535
I	6.295719	3.376903	3.746392	H	7.540102	4.395719	-0.925092
Se	1.920367	-1.063323	5.730675	H	8.441197	6.696944	0.733397
C	3.705937	-1.811571	6.011111	H	9.384029	5.258457	0.341820
H	0.284278	-0.396555	-1.317370	H	1.010363	1.965233	-2.512132
H	0.064238	-1.352933	0.961941	H	2.729678	2.314172	-2.256908

C	1.965346	1.536782	-2.190714	H	2.219681	0.743142	-2.900912

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.285726 hartree
Thermal correction to Gibbs free energy = 0.226289 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10208.6807505 hartree

TS1 of the reaction for 7a:

Atom	x	y	z	Atom	x	y	z
C	0.311824	-0.867659	0.023425	H	2.761894	1.395701	-0.656304
C	0.483606	-1.018520	1.374784	H	4.008304	1.955168	1.447640
C	1.498184	-0.292193	2.046018	H	4.006553	-2.182473	5.389491
C	2.326809	0.585857	1.298805	H	2.224837	-2.359284	5.224377
C	2.119802	0.719192	-0.097725	H	2.979106	-2.328817	6.851143
C	1.132103	0.010607	-0.740082	N	7.251956	4.651426	1.947259
C	3.343679	1.287615	1.990431	C	7.057335	4.789937	0.585103
N	1.636708	-0.452127	3.396744	C	8.262417	5.457984	2.438878
C	3.494842	1.104030	3.342030	C	8.050426	5.817094	0.054767
C	2.578379	0.208356	3.998793	O	6.228694	4.186763	-0.063212
C	4.517952	1.691895	4.176131	C	8.852669	6.255144	1.281284
C	4.786381	1.492401	5.384651	O	8.607612	5.508165	3.599647
H	5.296467	1.624702	6.319535	H	7.492326	6.631120	-0.413750
I	6.093098	3.327474	3.130105	H	8.659911	5.345812	-0.719763
Se	2.784285	-0.021206	5.902611	H	8.758505	7.319855	1.506947
C	3.037117	-1.956187	5.829534	H	9.918366	6.025526	1.208931
H	-0.467984	-1.426919	-0.486802	H	-0.118024	0.492848	-2.424262
H	-0.141696	-1.684624	1.959909	H	1.601873	0.842210	-2.674099
C	0.898420	0.140217	-2.221257	H	1.010975	-0.828732	-2.718384

Number of imaginary frequencies = 1 (-253.0563 cm^{-1})
Zero-point vibrational correction = 0.285032 hartree
Thermal correction to Gibbs free energy = 0.227738 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10208.6570801 hartree

IM of the reaction for 7a:

Atom	x	y	z	Atom	x	y	z
C	-0.048070	-1.131952	0.113793	H	2.379589	1.053864	-0.845199
C	0.181834	-1.182295	1.463673	H	3.710209	1.790188	1.139400
C	1.228227	-0.415474	2.030231	H	4.519508	-1.454350	4.949728
C	2.031982	0.401817	1.183979	H	3.026428	-2.215853	5.624468
C	1.761394	0.426855	-0.208047	H	4.265037	-1.535134	6.734438
C	0.742991	-0.321436	-0.749363	N	7.325877	4.646643	1.996614
C	3.079483	1.161658	1.763002	C	7.412240	4.843436	0.648582
N	1.432728	-0.479443	3.383624	C	8.221768	5.426079	2.669517
C	3.288776	1.087912	3.118709	C	8.500911	5.875043	0.321472

C	2.403290	0.237883	3.834744	O	6.726847	4.285707	-0.198570
C	4.311062	1.754814	3.928853	C	9.045007	6.273191	1.689047
C	4.288400	1.458360	5.235005	O	8.364674	5.460311	3.884674
H	4.920922	1.836535	6.025910	H	8.051563	6.702776	-0.233636
I	5.734296	3.111278	3.048315	H	9.245070	5.409999	-0.330732
Se	2.859143	0.266962	5.716162	H	8.903686	7.330477	1.928914
C	3.790803	-1.450600	5.758182	H	10.105573	6.045847	1.826132
H	-0.852287	-1.721551	-0.317882	H	-0.577850	0.039027	-2.407686
H	-0.419605	-1.797638	2.124136	H	1.130954	0.355463	-2.759816
C	0.445330	-0.304167	-2.224051	H	0.531810	-1.309835	-2.647779

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.287398 hartree
Thermal correction to Gibbs free energy = 0.231100 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10208.6902496 hartree

Reactant2 of the reaction for 7a:

Atom	x	y	z	Atom	x	y	z
C	-2.391899	-2.721200	-1.678081	H	0.378201	4.717064	0.671178
C	-2.809392	-1.519271	-1.169445	N	-2.310830	0.708910	-0.443537
C	-1.869338	-0.485466	-0.947572	Se	-1.841556	3.351133	0.461333
C	-0.495602	-0.711060	-1.258442	I	2.772950	2.857534	-0.465156
C	-0.104441	-1.968373	-1.784015	C	-0.627080	-4.307585	-2.548932
C	-1.025280	-2.967315	-1.995068	H	-0.880529	-5.105877	-1.844213
C	0.435949	0.330523	-1.027913	H	-1.162938	-4.514100	-3.480718
C	-0.014436	1.520397	-0.511910	H	0.445040	-4.352538	-2.749908
C	-1.407575	1.606456	-0.258285	H	-3.115510	-3.513594	-1.847888
C	0.024837	3.743550	0.363745	C	-1.998350	2.814069	2.335224
C	0.727646	2.730658	-0.160767	H	-1.132240	2.202751	2.581532
H	-3.849627	-1.329370	-0.928778	H	-2.040208	3.727878	2.925661
H	0.944344	-2.130414	-2.018014	H	-2.930590	2.254320	2.407285
H	1.488469	0.181174	-1.254188				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.206224 hartree
Thermal correction to Gibbs free energy = 0.162210 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -9848.50172721 hartree

Entrance2 of the reaction for 7a:

Atom	x	y	z	Atom	x	y	z
C	-2.582099	-2.828216	-2.329000	I	2.387520	3.004871	-1.590425
C	-2.918358	-1.753099	-1.549436	C	-1.468521	2.196989	2.305612
C	-2.015586	-0.671291	-1.413430	H	-0.563354	1.598408	2.230043
C	-0.762882	-0.718266	-2.092597	H	-1.351088	3.049125	2.984693
C	-0.453116	-1.848497	-2.891580	H	-2.336436	1.595630	2.571292

C	-1.336834	-2.893743	-3.017339	C	-0.883414	1.125211	6.274322
C	0.132585	0.368986	-1.944453	C	-0.953362	3.183393	5.463506
C	-0.235919	1.427083	-1.151626	N	-1.008216	1.871907	5.140925
C	-1.515595	1.344645	-0.541134	C	-0.720053	2.003366	7.530757
C	-0.106926	3.508736	0.010283	H	0.221896	1.750464	8.025669
C	0.497416	2.646948	-0.817241	H	-1.527494	1.777724	8.233171
H	-3.276869	-3.657316	-2.431017	C	-0.765127	3.417496	6.972041
H	-3.865700	-1.699819	-1.024179	H	0.152135	3.990594	7.135500
H	0.503913	-1.874979	-3.405968	H	-1.596571	4.019872	7.349266
C	-1.022445	-4.100086	-3.859067	O	-1.041639	4.128069	4.666161
H	1.094412	0.357058	-2.450694	O	-0.895014	-0.102510	6.331305
H	0.261968	4.457340	0.373023	H	-1.775691	-4.231070	-4.642454
N	-2.380106	0.393657	-0.634635	H	-0.043321	-4.009656	-4.333690
Se	-1.850549	2.924427	0.519589	H	-1.027439	-5.008361	-3.248063

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.287327 hartree
Thermal correction to Gibbs free energy = 0.229009 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10208.6795551 hartree

TS2 of the reaction for 7a:

Atom	x	y	z	Atom	x	y	z
C	-2.594306	-2.817984	-1.672908	I	2.457484	2.995972	-1.616077
C	-2.945397	-1.626691	-1.096569	C	-1.471599	2.655012	2.332443
C	-2.027661	-0.546733	-1.086421	H	-0.500776	2.206549	2.169623
C	-0.743268	-0.722118	-1.680297	H	-1.515640	3.612967	2.839310
C	-0.418083	-1.972679	-2.268506	H	-2.314337	1.985314	2.445878
C	-1.316074	-3.011799	-2.273076	C	-0.834175	0.989193	5.256746
C	0.166930	0.360117	-1.658907	C	-1.095802	3.210963	5.314757
C	-0.218377	1.540169	-1.070225	N	-1.069112	2.111843	4.519517
C	-1.531911	1.582454	-0.524081	C	-0.676700	1.334231	6.748184
C	-0.116691	3.774833	-0.256699	H	0.302705	0.991102	7.092307
C	0.521370	2.784676	-0.898157	H	-1.432897	0.789938	7.320480
H	-3.301306	-3.643183	-1.677373	C	-0.848427	2.848420	6.786230
H	-3.917064	-1.476409	-0.638680	H	0.034948	3.385010	7.143273
H	0.563934	-2.094734	-2.718252	H	-1.698875	3.183817	7.386057
C	-0.985824	-4.343206	-2.890951	O	-1.291833	4.363164	4.925443
H	1.154830	0.250603	-2.099169	O	-0.754328	-0.153006	4.819607
H	0.256982	4.764712	-0.037321	H	-1.697451	-4.588322	-3.685904
N	-2.408465	0.631312	-0.508508	H	0.019877	-4.345162	-3.316437
Se	-1.879837	3.297312	0.260819	H	-1.045682	-5.141368	-2.144071

Number of imaginary frequencies = 1 (-449.5897 cm^{-1})
Zero-point vibrational correction = 0.286973 hartree
Thermal correction to Gibbs free energy = 0.230142 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10208.6705897 hartree

Product of the reaction for 7a:

Atom	x	y	z	Atom	x	y	z
C	-2.330403	-2.763682	-1.638224	H	0.951853	-2.088438	-2.237973
C	-2.721298	-1.591903	-1.052284	H	1.509810	0.213232	-1.435490
C	-1.787970	-0.534749	-0.867148	H	0.449929	4.648377	0.677668
C	-0.443040	-0.724702	-1.303619	N	-2.214439	0.615319	-0.280772
C	-0.076907	-1.959288	-1.909846	Se	-1.728395	3.231585	0.667455
C	-0.988671	-2.968598	-2.081550	I	2.806503	2.892770	-0.666271
C	0.476966	0.326713	-1.114720	C	-0.615644	-4.279251	-2.720735
C	0.048449	1.492621	-0.520252	H	-0.793938	-5.112348	-2.032843
C	-1.326006	1.559541	-0.128167	H	-1.220922	-4.462608	-3.614615
C	0.074243	3.680554	0.376109	H	0.437297	-4.294006	-3.010890
C	0.783772	2.701595	-0.215792	H	-3.051016	-3.565860	-1.774979
H	-3.740247	-1.433869	-0.714496				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.167774 hartree
Thermal correction to Gibbs free energy = 0.126353 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -9808.82077385 hartree

Reaction for 7b

Reactant1 of the reaction for 7b:

Atom	x	y	z	Atom	x	y	z
C	-2.230724	-4.037863	-1.453663	H	0.580911	-0.275461	-2.833770
C	-2.337114	-3.013326	-0.543047	N	-1.744490	-0.830173	0.232632
C	-1.610503	-1.808099	-0.711649	Se	-1.357761	1.630712	1.426741
C	-0.762081	-1.657089	-1.838701	H	-1.293761	-4.687346	-3.297254
C	-0.660066	-2.721975	-2.772156	C	-2.994396	-5.324317	-1.288972
C	-1.374121	-3.874349	-2.580506	H	-3.649455	-5.499057	-2.148711
C	-0.066258	-0.437125	-1.976196	H	-2.309568	-6.176239	-1.225271
C	-0.222941	0.555402	-1.032274	H	-3.608647	-5.308520	-0.386195
C	-1.085097	0.286947	0.083946	H	1.537746	3.785965	-1.492890
C	1.029599	2.856344	-1.352385	C	0.447829	1.633594	2.167779
C	0.445506	1.813062	-1.185829	H	0.438694	2.362978	2.978154
H	-2.977982	-3.099630	0.329599	H	1.167229	1.933873	1.407117
H	-2.230724	-2.605286	-3.635366	H	0.672253	0.644491	2.562923

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.202274 hartree
Thermal correction to Gibbs free energy = 0.160197 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -2958.16193836 hartree

Entrance1 of the reaction for 7b:

Atom	x	y	z	Atom	x	y	z
C	0.928920	-0.071944	-0.540447	H	3.424114	2.214938	0.026312
C	0.811154	-0.588273	0.728818	H	4.068756	2.170752	2.435583
C	1.627479	-0.113756	1.785569	H	4.424424	-0.996555	6.191199
C	2.573253	0.909643	1.527578	H	3.996513	-2.414496	5.175650
C	2.691079	1.434628	0.213302	H	3.626185	-2.417982	6.917867
C	1.888688	0.952639	-0.786469	N	7.047074	4.321780	2.122789
C	3.352444	1.373414	2.607475	C	6.418841	4.233651	0.883489
N	1.487050	-0.672763	3.023537	C	8.208037	5.096648	2.119597
C	3.187819	0.823593	3.862707	C	7.236196	5.044508	-0.105677
C	2.230566	-0.239800	4.006458	O	5.403538	3.611754	0.673567
C	3.925136	1.322918	4.987609	C	8.409455	5.608227	0.703314
C	4.537513	1.751668	5.939440	O	8.896722	5.297132	3.088508
H	5.047776	2.111290	6.808266	H	6.593507	5.817578	-0.532715
I	6.297316	3.382966	3.754608	H	7.547733	4.385132	-0.918800
Se	1.917901	-1.067289	5.716091	H	8.431343	6.699865	0.730431
C	3.706323	-1.797283	6.024725	H	9.383663	5.265145	0.348009
H	0.928920	-0.071944	-1.793166	H	-0.615169	-1.346618	-1.343882
H	0.811154	-0.588273	0.953845	H	-0.519208	0.255541	-2.097943
C	1.627479	-0.113756	-1.674891	H	0.690330	-0.967345	-2.482713

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.285690 hartree
Thermal correction to Gibbs free energy = 0.226041 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10208.6812660 hartree

TS1 of the reaction for 7b:

Atom	x	y	z	Atom	x	y	z
C	0.301986	-0.895024	0.014430	H	2.763662	1.386149	-0.672547
C	0.494832	-1.025000	1.370168	H	4.018362	1.958373	1.441070
C	1.508340	-0.293341	2.035179	H	3.984719	-2.191020	5.391808
C	2.339883	0.586929	1.293199	H	2.201343	-2.346028	5.222276
C	2.128581	0.712895	-0.104255	H	2.951694	-2.319993	6.851219
C	1.139429	-0.007688	-0.719665	N	7.260038	4.657105	1.950805
C	3.353939	1.290546	1.983851	C	7.069115	4.795460	0.588199
N	1.645780	-0.450601	3.387440	C	8.268385	5.464553	2.445072
C	3.503358	1.108407	3.336396	C	8.062708	5.823525	0.060450
C	2.585770	0.212214	3.989529	O	6.242802	4.191611	-0.062547
C	4.524104	1.696362	4.172892	C	8.861383	6.262087	1.289086
C	4.789799	1.494493	5.382026	O	8.610355	5.515272	3.606818
H	5.297953	1.626963	6.317945	H	7.505113	6.637133	-0.409400
I	6.098670	3.331572	3.131033	H	8.674563	5.352861	-0.712588
Se	2.787562	-0.013386	5.894655	H	8.766085	7.326757	1.514465

C	3.017008	-1.951520	5.828573	H	9.927393	6.033005	1.219623
H	0.982688	0.092593	-1.790215	H	-1.331656	-2.303242	-0.022517
H	-0.124675	-1.688776	1.965891	H	-1.473596	-0.982253	-1.197068
C	-0.770694	-1.664500	-0.707994	H	-0.334926	-2.295528	-1.489399

Number of imaginary frequencies = 1 (-253.1966 cm^{-1})
Zero-point vibrational correction = 0.285016 hartree
Thermal correction to Gibbs free energy = 0.227771 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10208.6573291 hartree

IM of the reaction for 7b:

Atom	x	y	z	Atom	x	y	z
C	-0.055471	-1.163650	0.112005	H	2.381558	1.041074	-0.857501
C	0.195358	-1.191117	1.464187	H	3.719915	1.793314	1.135687
C	1.239093	-0.417613	2.023602	H	4.524178	-1.442097	4.955833
C	2.045819	0.402086	1.182074	H	3.026823	-2.204269	5.620456
C	1.771336	0.418069	-0.210631	H	4.258685	-1.524832	6.738799
C	0.753729	-0.341513	-0.723079	N	7.334642	4.656453	2.004167
C	3.089282	1.165021	1.759710	C	7.424264	4.853166	0.656380
N	1.441740	-0.476808	3.378918	C	8.232027	5.432633	2.678746
C	3.295927	1.094954	3.116860	C	8.516209	5.882022	0.331437
C	2.409283	0.244596	3.829769	O	6.739304	4.297105	-0.192218
C	4.314402	1.764257	3.928922	C	9.060407	6.276660	1.699949
C	4.288396	1.470147	5.235724	O	8.372347	5.466746	3.894200
H	4.917700	1.851032	6.027837	H	8.069371	6.711938	-0.222461
I	5.739308	3.120373	3.051235	H	9.259439	5.416112	-0.321178
Se	2.859080	0.278318	5.713780	H	8.924294	7.334469	1.940431
C	3.790461	-1.439270	5.759752	H	10.119618	6.043701	1.838163
H	0.551133	-0.323113	-1.790308	H	-0.760153	-2.669440	-1.251040
H	-0.399142	-1.803299	2.135441	H	-1.695140	-2.557736	0.252285
C	-1.160765	-1.977837	-0.502909	H	-1.879548	-1.328740	-1.013278

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.287347 hartree
Thermal correction to Gibbs free energy = 0.230916 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10208.6903813 hartree

Reactant2 of the reaction for 7b:

Atom	x	y	z	Atom	x	y	z
C	-2.379832	-4.196236	-1.628424	N	-2.416066	-0.849063	-0.155170
C	-2.753610	-3.104033	-0.879404	Se	-2.124001	1.806654	0.786402
C	-1.995059	-1.912150	-0.912184	I	1.821862	2.292432	-1.776668
C	-0.825988	-1.833779	-1.726332	H	-0.925366	-4.975122	-3.031826
C	-0.457882	-2.969454	-2.493864	C	-3.171619	-5.474196	-1.610997
C	-1.213812	-4.109784	-2.441992	H	-3.541476	-5.709950	-2.614018

C	-0.075521	-0.635179	-1.738539	H	-2.542899	-6.311494	-1.291862
C	-0.497835	0.418440	-0.964631	H	-4.025854	-5.404712	-0.934952
C	-1.683444	0.206607	-0.215526	H	-0.261637	3.585515	0.333111
C	-0.527213	2.571117	0.072936	C	-1.496662	1.202764	2.537217
C	0.094986	1.740922	-0.775055	H	-0.504542	0.774241	2.411235
H	-3.636396	-3.127656	-0.248305	H	-1.489741	2.075325	3.188268
H	0.428866	-2.917354	-3.117930	H	-2.223711	0.464625	2.875377
H	0.820048	-0.557586	-2.349615				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.206228 hartree
Thermal correction to Gibbs free energy = 0.162021 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -9848.50210308 hartree

Entrance2 of the reaction for 7b:

Atom	x	y	z	Atom	x	y	z
C	-2.581847	-2.860626	-2.293585	I	2.380689	3.029479	-1.617031
C	-2.895684	-1.766679	-1.521133	C	-1.448198	2.197270	2.303857
C	-1.994718	-0.683633	-1.399479	H	-0.537402	1.607685	2.225104
C	-0.743510	-0.720046	-2.082730	H	-1.337681	3.049853	2.983451
C	-0.437833	-1.856598	-2.876651	H	-2.309358	1.587016	2.571304
C	-1.331049	-2.889397	-2.974633	C	-0.869809	1.126219	6.273548
C	0.145394	0.371399	-1.945158	C	-0.954996	3.184734	5.465028
C	-0.225840	1.431538	-1.154852	N	-0.990699	1.873194	5.139924
C	-1.501706	1.340570	-0.538812	C	-0.729957	2.004183	7.532920
C	-0.106496	3.518077	-0.000606	H	0.209854	1.761525	8.036930
C	0.499341	2.657861	-0.828941	H	-1.541737	1.767916	8.226775
H	-1.089482	-3.756188	-3.583330	C	-0.785870	3.418581	6.975891
H	-3.838205	-1.705063	-0.986208	H	0.122537	4.002434	7.150265
H	0.512738	-1.891189	-3.400128	H	-1.628570	4.010246	7.344974
C	-3.524845	-4.023248	-2.436082	O	-1.046204	4.129576	4.668235
H	1.104637	0.362728	-2.456437	O	-0.868385	-0.101641	6.328755
H	0.256730	4.471200	0.355808	H	-4.440455	-3.865489	-1.862824
N	-2.360987	0.384254	-0.622741	H	-3.794562	-4.173435	-3.486366
Se	-1.842690	2.921957	0.519437	H	-3.052203	-4.946834	-2.086886

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.287240 hartree
Thermal correction to Gibbs free energy = 0.228536 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10208.6799417 hartree

TS2 of the reaction for 7b:

Atom	x	y	z	Atom	x	y	z
C	-2.587239	-2.852762	-1.628014	I	2.452740	3.014731	-1.613650
C	-2.921916	-1.644004	-1.065904	C	-1.476095	2.655891	2.330941

C	-2.007148	-0.563210	-1.065321	H	-0.500079	2.218009	2.170221
C	-0.718860	-0.728118	-1.654667	H	-1.531306	3.613549	2.837257
C	-0.391107	-1.984627	-2.231296	H	-2.311504	1.976935	2.443808
C	-1.298085	-3.008804	-2.216099	C	-0.818995	0.999457	5.256681
C	0.183418	0.358531	-1.640583	C	-1.104389	3.218291	5.313290
C	-0.211135	1.540752	-1.060734	N	-1.069491	2.118561	4.519237
C	-1.525614	1.574477	-0.517442	C	-0.659335	1.347838	6.747110
C	-0.128350	3.780862	-0.260189	H	0.325157	1.015866	7.087635
C	0.517938	2.791917	-0.895445	H	-1.407210	0.795930	7.323032
H	-1.039677	-3.966791	-2.658617	C	-0.847497	2.860099	6.784206
H	-3.893078	-1.485007	-0.607521	H	0.031245	3.406768	7.137367
H	0.588705	-2.115027	-2.680877	H	-1.699325	3.186789	7.386877
C	-3.545448	-4.012086	-1.636458	O	-1.313712	4.367968	4.923434
H	1.172670	0.252258	-2.078756	O	-0.728152	-0.142275	4.820441
H	0.236824	4.775099	-0.046552	H	-4.493285	-3.747845	-1.163304
N	-2.395997	0.617869	-0.495875	H	-3.748732	-4.337370	-2.661839
Se	-1.887800	3.291241	0.258265	H	-3.119460	-4.867902	-1.102903

Number of imaginary frequencies = 1 (-448.9543 cm^{-1})
Zero-point vibrational correction = 0.286951 hartree
Thermal correction to Gibbs free energy = 0.229997 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10208.6710025 hartree

Product of the reaction for 7b:

Atom	x	y	z	Atom	x	y	z
C	-2.331673	-4.211718	-1.644295	H	0.350464	-2.877173	-3.306422
C	-2.653576	-3.141529	-0.848782	H	0.769683	-0.525356	-2.520523
C	-1.909771	-1.931278	-0.902998	N	-2.281227	-0.906896	-0.088785
C	-0.806496	-1.831831	-1.802740	Se	-1.941691	1.720320	0.889026
C	-0.488708	-2.953088	-2.620678	I	1.774143	2.335912	-1.986171
C	-1.226758	-4.100321	-2.542085	H	-0.976966	-4.951081	-3.170288
C	-0.076383	-0.628002	-1.845034	C	-3.111688	-5.497848	-1.595918
C	-0.450581	0.410234	-1.020630	H	-3.545117	-5.725404	-2.575442
C	-1.575141	0.188765	-0.164631	H	-2.460551	-6.336436	-1.327886
C	-0.477983	2.529082	0.028569	H	-3.921843	-5.444221	-0.865493
C	0.123812	1.730395	-0.872422	H	-0.193123	3.542427	0.274666
H	-3.486992	-3.187758	-0.153911				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.167760 hartree
Thermal correction to Gibbs free energy = 0.126344 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -9808.82122858 hartree

Reaction for 7c

Reactant1 of the reaction for 7c:

Atom	x	y	z	Atom	x	y	z
C	-2.314008	-2.637903	-1.381274	H	-3.562545	-1.409844	-0.128103
C	-2.611690	-1.522838	-0.638271	H	0.834133	-1.839292	-2.433366
C	-1.663860	-0.476221	-0.518129	H	-0.846200	-3.647217	-2.617808
C	-0.410069	-0.594811	-1.173430	H	1.465853	0.434302	-1.535516
C	-0.127575	-1.757979	-1.934858	H	2.537238	4.416566	-0.053498
C	-1.061800	-2.757647	-2.035143	N	-1.989220	0.612864	0.240309
C	0.501169	0.477008	-1.037592	Se	-1.671229	3.102106	1.395273
C	0.158527	1.581969	-0.290184	C	-0.386541	2.893920	2.849725
C	-1.127095	1.585615	0.352566	H	-0.593177	3.703205	3.550498
C	1.848063	3.602018	-0.115145	H	0.630487	2.983249	2.470216
C	1.058871	2.691087	-0.182096	H	-0.550283	1.933435	3.334955
H	-3.040731	-3.438763	-1.472219				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.174556 hartree
Thermal correction to Gibbs free energy = 0.134740 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -2918.85382758 hartree

Entrance1 of the reaction for 7c:

Atom	x	y	z	Atom	x	y	z
C	0.922061	-0.034885	-0.522163	H	1.957973	1.390248	-1.785257
C	0.791680	-0.569571	0.735818	H	3.412245	2.239265	0.043868
C	1.611939	-0.100259	1.791717	H	4.058783	2.179263	2.442192
C	2.557708	0.923960	1.531824	H	4.426130	-1.006673	6.178386
C	2.677113	1.459226	0.223081	H	3.988157	-2.421272	5.162126
C	1.871930	0.985483	-0.782256	H	3.627801	-2.427302	6.906479
C	3.342182	1.381982	2.613292	N	7.047249	4.311881	2.116930
N	1.475651	-0.664303	3.028420	C	6.409309	4.229992	0.882239
C	3.181550	0.827141	3.865249	C	8.212515	5.080410	2.106831
C	2.222826	-0.236927	4.009738	C	7.223804	5.038319	-0.111282
C	3.923882	1.320424	4.989689	O	5.388993	3.614225	0.678780
C	4.539930	1.743670	5.941417	C	8.406371	5.593499	0.690052
H	5.054301	2.098796	6.809706	O	8.909140	5.275198	3.071145
I	6.304555	3.373947	3.752164	H	6.582353	5.816060	-0.531667
Se	1.916460	-1.069480	5.717754	H	7.525313	4.379032	-0.928233
C	3.704750	-1.804963	6.014182	H	8.435103	6.684924	0.718980
H	0.294433	-0.395532	-1.330741	H	9.375791	5.245143	0.326870
H	0.074353	-1.353325	0.955110				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.257929 hartree
Thermal correction to Gibbs free energy = 0.200522 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10166.272358 hartree

TS1 of the reaction for 7c:

Atom	x	y	z	Atom	x	y	z
C	0.321015	-0.874165	0.013054	H	0.992763	0.107937	-1.798690
C	0.494811	-1.021056	1.367349	H	2.775798	1.398511	-0.665860
C	1.508119	-0.291102	2.034232	H	4.020044	1.960580	1.444491
C	2.339884	0.589691	1.291330	H	3.987722	-2.190822	5.387452
C	2.136261	0.723072	-0.105383	H	2.204343	-2.350568	5.221038
C	1.146938	0.005107	-0.729803	H	2.957549	-2.323709	6.848552
C	3.354918	1.292424	1.985916	N	7.259229	4.656578	1.951886
N	1.644951	-0.450084	3.386887	C	7.066190	4.795166	0.589483
C	3.503035	1.108317	3.336951	C	8.268558	5.463738	2.444943
C	2.584152	0.210883	3.990203	C	8.059079	5.823249	0.060642
C	4.523741	1.694950	4.174671	O	6.238817	4.191449	-0.059941
C	4.787481	1.490330	5.383716	C	8.859849	6.261263	1.288149
H	5.296118	1.620507	6.319757	O	8.612124	5.513975	3.606172
I	6.099696	3.331715	3.132634	H	7.500818	6.637137	-0.407929
Se	2.785953	-0.016828	5.894908	H	8.669601	5.352843	-0.713598
C	3.020110	-1.954356	5.826055	H	8.765270	7.325914	1.513896
H	-0.456059	-1.433879	-0.497083	H	9.925662	6.031826	1.216899
H	-0.127511	-1.685892	1.956863				

Number of imaginary frequencies = 1 (-252.2218 cm^{-1})
Zero-point vibrational correction = 0.257250 hartree
Thermal correction to Gibbs free energy = 0.202220 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10169.3491119 hartree

IM of the reaction for 7c:

Atom	x	y	z	Atom	x	y	z
C	-0.031836	-1.137946	0.089788	H	0.569726	-0.304854	-1.817949
C	0.196893	-1.182366	1.442866	H	2.402965	1.055655	-0.866667
C	1.240439	-0.411430	2.006243	H	3.727981	1.796593	1.127484
C	2.049991	0.407411	1.165192	H	4.515900	-1.444993	4.946849
C	1.785994	0.430793	-0.228198	H	3.016253	-2.204894	5.609305
C	0.767822	-0.325793	-0.751708	H	4.247031	-1.526393	6.729369
C	3.094515	1.168663	1.748944	N	7.338128	4.655904	2.008488
N	1.439582	-0.472316	3.362476	C	7.431105	4.853558	0.660939
C	3.296783	1.096537	3.105165	C	8.230876	5.434685	2.686480
C	2.406389	0.246299	3.816626	C	8.520684	5.886038	0.340112
C	4.314509	1.763706	3.920446	O	6.750312	4.295698	-0.189689
C	4.284021	1.468153	5.226605	C	9.059338	6.281772	1.710547
H	4.912097	1.846916	6.020792	O	8.367118	5.468418	3.902308
I	5.744216	3.119609	3.047178	H	8.072915	6.714804	-0.214741
Se	2.851606	0.277984	5.701661	H	9.267482	5.422885	-0.310371
C	3.780699	-1.440862	5.749399	H	8.919006	7.339006	1.951073

H	-0.832131	-1.728575	-0.343318	H	10.118870	6.052208	1.851898
H	-0.402943	-1.795278	2.106847				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.259600 hartree
Thermal correction to Gibbs free energy = 0.205363 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10169.3818678 hartree

Reactant2 of the reaction for 7c:

Atom	x	y	z	Atom	x	y	z
C	-2.393192	-2.745301	-1.633368	H	-3.847699	-1.337318	-0.897309
C	-2.808412	-1.534833	-1.135430	H	0.952823	-2.156234	-1.971334
C	-1.865448	-0.503446	-0.922723	H	-0.724208	-3.937748	-2.330709
C	-0.488699	-0.726909	-1.226077	H	1.494621	0.167142	-1.221596
C	-0.094432	-1.988259	-1.740123	H	0.368860	4.718756	0.658750
C	-1.028477	-2.973792	-1.937753	N	-2.309105	0.697512	-0.430761
C	0.441155	0.317912	-1.000719	Se	-1.847927	3.348121	0.450674
C	-0.012366	1.511175	-0.497194	I	2.772378	2.852906	-0.447908
C	-1.407790	1.596487	-0.251079	C	-2.013709	2.822453	2.327083
C	0.018494	3.741885	0.358580	H	-1.145653	2.217781	2.582710
C	0.725888	2.725709	-0.153232	H	-2.064670	3.739754	2.911280
H	-3.114926	-3.538168	-1.797645	H	-2.943173	2.257703	2.396340

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.178529 hartree
Thermal correction to Gibbs free energy = 0.136834 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -9809.19322428 hartree

Entrance2 of the reaction for 7c:

Atom	x	y	z	Atom	x	y	z
C	-2.564809	-2.849246	-2.298430	Se	-1.842149	2.924031	0.512945
C	-2.898429	-1.766442	-1.523374	I	2.384626	3.021765	-1.619833
C	-1.996555	-0.683718	-1.401957	C	-1.451100	2.201936	2.299720
C	-0.744878	-0.724647	-2.085560	H	-0.541507	1.610268	2.223463
C	-0.432423	-1.857844	-2.879405	H	-1.339648	3.056110	2.977256
C	-1.324106	-2.895501	-2.981354	H	-2.314178	1.594376	2.567016
C	0.145646	0.368608	-1.947073	C	-0.876889	1.119305	6.260906
C	-0.225116	1.428391	-1.158815	C	-0.957692	3.180757	5.459279
C	-1.502760	1.340736	-0.542634	N	-0.994740	1.870375	5.129609
C	-0.104023	3.515637	-0.006735	C	-0.738592	1.992758	7.523556
C	0.501986	2.654314	-0.833545	H	0.199375	1.746607	8.029294
H	-3.255278	-3.680630	-2.391808	H	-1.552727	1.755661	8.214392
H	-3.841795	-1.708559	-0.991715	C	-0.790565	3.409146	6.971193
H	0.520207	-1.887205	-3.399248	H	0.118925	3.990314	7.148966
H	-1.081541	-3.761040	-3.588294	H	-1.632500	4.001502	7.340934

H	1.105369	0.358614	-2.457342	O	-1.046206	4.128440	4.665544
H	0.260464	4.468476	0.349363	O	-0.877045	-0.108710	6.311774
N	-2.362228	0.385756	-0.626472				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.259565 hartree
Thermal correction to Gibbs free energy = 0.203382 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10169.3712277 hartree

TS2 of the reaction for 7c:

Atom	x	y	z	Atom	x	y	z
C	-2.565896	-2.840056	-1.654055	Se	-1.885665	3.287786	0.255449
C	-2.920892	-1.644078	-1.083294	I	2.455995	3.013014	-1.616702
C	-2.006259	-0.562942	-1.079739	C	-1.476118	2.650134	2.326248
C	-0.718158	-0.728772	-1.670961	H	-0.502629	2.206372	2.166288
C	-0.383383	-1.979291	-2.253568	H	-1.525251	3.607757	2.833464
C	-1.287734	-3.009686	-2.244449	H	-2.315145	1.975893	2.440675
C	0.184858	0.360284	-1.652562	C	-0.834614	0.989627	5.256583
C	-0.209246	1.539108	-1.069157	C	-1.102896	3.210601	5.309371
C	-1.524801	1.572783	-0.524767	N	-1.072346	2.109862	4.516588
C	-0.125281	3.776396	-0.261793	C	-0.679154	1.338444	6.747348
C	0.521029	2.789588	-0.899965	H	0.300941	0.998802	7.092964
H	-3.266974	-3.667985	-1.655485	H	-1.434264	0.793366	7.320336
H	-3.892230	-1.491844	-0.625611	C	-0.855163	2.852230	6.781807
H	0.597861	-2.101114	-2.702206	H	0.026562	3.392116	7.137968
H	-1.028250	-3.963987	-2.690001	H	-1.706784	3.186650	7.380510
H	1.174014	0.255344	-2.091114	O	-1.302360	4.361357	4.917374
H	0.240655	4.769703	-0.044827	O	-0.751131	-0.153351	4.822106
N	-2.394632	0.616898	-0.506329				

Number of imaginary frequencies = 1 (-447.0127 cm^{-1})
Zero-point vibrational correction = 0.259222 hartree
Thermal correction to Gibbs free energy = 0.204601 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10169.3624891 hartree

Product of the reaction for 7c:

Atom	x	y	z	Atom	x	y	z
C	-2.406690	-2.719690	-1.610561	C	0.748238	2.738260	-0.217026
C	-2.809949	-1.493294	-1.152921	H	-3.138108	-3.504406	-1.774570
C	-1.858505	-0.460045	-0.935299	H	-3.851767	-1.273376	-0.944616
C	-0.479501	-0.719405	-1.199865	H	0.955891	-2.192676	-1.873365
C	-0.095361	-2.004476	-1.674503	H	-0.736835	-3.957992	-2.236879
C	-1.035032	-2.979711	-1.874833	H	1.510754	0.146396	-1.170834
C	0.453769	0.314879	-0.978855	H	0.389039	4.753748	0.494806
C	0.006627	1.532396	-0.519034	N	-2.301957	0.743431	-0.480342

C	-1.400748	1.667829	-0.292134	Se	-1.825706	3.403833	0.337144
C	0.013804	3.777498	0.221307	I	2.813613	2.838400	-0.449898

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.139960 hartree
Thermal correction to Gibbs free energy = 0.100712 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -9769.51311574 hartree

Reaction for 7d

Reactant1 of the reaction for 7d:

Atom	x	y	z	Atom	x	y	z
C	-2.174301	-2.760161	-1.284545	H	0.854466	-1.892254	-2.573443
C	-2.432568	-1.665956	-0.501333	H	1.502635	0.387571	-1.719803
C	-1.498242	-0.600595	-0.437630	Br	2.963808	5.021229	-0.344979
C	-0.304433	-0.691571	-1.197629	N	-1.771516	0.466149	0.366212
C	-0.066198	-1.839407	-1.997245	Se	-1.466987	2.919141	1.537627
C	-0.977469	-2.866454	-2.050325	C	-0.744869	-4.092087	-2.892658
C	0.589986	0.398932	-1.130683	H	0.209262	-4.035051	-3.421216
C	0.294281	1.492751	-0.344333	H	-0.740854	-4.994777	-2.273023
C	-0.920951	1.456419	0.422691	H	-1.541710	-4.211452	-3.634008
C	1.894174	3.587823	-0.358304	C	0.181151	3.291126	2.527700
C	1.158372	2.629426	-0.340674	H	-0.127832	3.593645	3.528299
H	-2.893871	-3.573585	-1.328922	H	0.755303	4.081325	2.048945
H	-3.341875	-1.584134	0.084797	H	0.772100	2.377540	2.591381

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.194062 hartree
Thermal correction to Gibbs free energy = 0.148802 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -5519.60652334 hartree

Entrance1 of the reaction for 7d:

Atom	x	y	z	Atom	x	y	z
C	1.003425	0.108057	-0.631945	H	3.659420	2.130589	0.058921
C	0.795309	-0.453943	0.600517	H	4.243944	1.945456	2.483459
C	1.626670	-0.097058	1.692917	H	3.904759	-0.982089	6.887393
C	2.664270	0.846770	1.481766	H	4.149384	-1.887284	5.364512
C	2.856588	1.409543	0.192644	H	3.354860	-2.679658	6.745272
C	2.044721	1.053938	-0.857730	N	7.135573	4.428328	2.238538
C	3.456845	1.202580	2.595339	C	6.410540	4.107732	1.095286
N	1.410805	-0.687147	2.903739	C	8.197279	5.310430	2.008684
C	3.208768	0.628556	3.825510	C	7.032418	4.852801	-0.070986
C	2.166297	-0.353409	3.916281	O	5.458405	3.363523	1.071500

C	3.965031	1.061642	4.956771	C	8.206262	5.635329	0.525570
C	4.642452	1.493814	5.858593	O	8.945286	5.712702	2.862872
Br	5.696085	2.173151	7.137800	H	6.267646	5.492643	-0.516904
I	6.693137	3.682179	4.067375	H	7.335628	4.122434	-0.824367
Se	1.718799	-1.206916	5.575106	H	8.110251	6.716879	0.408572
C	3.491125	-1.734458	6.219735	H	9.174644	5.341026	0.115011
H	0.363000	-0.169341	-1.465401	H	1.320882	2.159752	-2.558483
H	0.004515	-1.176487	0.773314	H	3.057597	2.346322	-2.255794
C	2.226837	1.637471	-2.233632	H	2.427404	0.850191	-2.967811

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.277087 hartree
Thermal correction to Gibbs free energy = 0.213951 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12770.1244888 hartree

TS1 of the reaction for 7d:

Atom	x	y	z	Atom	x	y	z
C	0.197394	-0.894536	-0.090251	H	2.648572	1.392029	-0.686647
C	0.339208	-1.060383	1.262807	H	3.820509	1.955101	1.458126
C	1.332976	-0.334887	1.965305	H	4.682502	-1.247515	5.232608
C	2.172484	0.556762	1.248561	H	3.318479	-2.417335	5.261381
C	1.998813	0.704422	-0.151010	H	4.043439	-1.844936	6.793951
C	1.030284	-0.002581	-0.823836	N	7.175462	4.533606	2.021016
C	3.157623	1.266450	1.975357	C	7.012097	4.733395	0.661927
N	1.445650	-0.517460	3.315769	C	8.251614	5.224539	2.549782
C	3.270155	1.081558	3.331805	C	8.103177	5.680349	0.177051
C	2.358901	0.150954	3.954282	O	6.140792	4.229804	-0.014261
C	4.229642	1.738209	4.185810	C	8.922427	6.007092	1.426852
C	4.399848	1.666581	5.430434	O	8.588866	5.199259	3.713457
Br	5.219169	2.074978	6.972510	H	7.629812	6.555111	-0.274914
I	5.892825	3.284032	3.149442	H	8.679779	5.176805	-0.602417
Se	2.511839	-0.103029	5.859838	H	8.913222	7.067751	1.688553
C	3.792571	-1.577775	5.767643	H	9.966381	5.692555	1.358367
H	-0.566917	-1.451959	-0.625247	H	-0.183019	0.498721	-2.528537
H	-0.294182	-1.737883	1.825672	H	1.541603	0.851930	-2.737272
C	0.829149	0.144237	-2.308081	H	0.952916	-0.818850	-2.813762

Number of imaginary frequencies = 1 (-266.7131 cm^{-1})
Zero-point vibrational correction = 0.275510 hartree
Thermal correction to Gibbs free energy = 0.214373 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12770.1056180 hartree

IM of the reaction for 7d:

Atom	x	y	z	Atom	x	y	z
C	-0.073546	-1.054132	0.058410	H	2.344258	1.169721	-0.837298

C	0.167743	-1.155571	1.403417	H	3.684139	1.839119	1.163484
C	1.217752	-0.408717	1.989232	H	4.531802	-1.510235	4.873702
C	2.013975	0.441300	1.168613	H	3.161405	-2.306726	5.742848
C	1.732188	0.518281	-0.219141	H	4.448913	-1.468766	6.676052
C	0.709638	-0.210188	-0.779619	N	7.286482	4.606671	1.999558
C	3.062118	1.183998	1.767824	C	7.353915	4.802664	0.649408
N	1.432887	-0.520191	3.337549	C	8.194343	5.383153	2.662359
C	3.282876	1.064613	3.119276	C	8.437194	5.834760	0.309897
C	2.405194	0.181127	3.807239	O	6.657219	4.243720	-0.186636
C	4.308906	1.718544	3.934148	C	9.005094	6.226934	1.669842
C	4.277506	1.385833	5.231064	O	8.352701	5.414705	3.874681
Br	5.390434	1.941012	6.613218	H	7.978041	6.665521	-0.232503
I	5.733877	3.084503	3.052457	H	9.169714	5.373333	-0.357695
Se	2.854240	0.169686	5.691127	H	8.874680	7.284515	1.914013
C	3.881312	-1.489395	5.746068	H	10.066153	5.992093	1.789006
H	-0.881041	-1.627489	-0.388653	H	-0.625898	0.213869	-2.410596
H	-0.427630	-1.795984	2.045258	H	1.079834	0.543331	-2.766016
C	0.398786	-0.136276	-2.249766	H	0.480818	-1.124959	-2.712542

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.277057 hartree
Thermal correction to Gibbs free energy = 0.217676 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12770.1372264 hartree

Reactant2 of the reaction for 7d:

Atom	x	y	z	Atom	x	y	z
C	-2.361645	-2.813988	-1.639461	H	1.429436	0.225704	-1.417798
C	-2.786109	-1.640634	-1.073312	Br	0.514715	5.348163	0.984061
C	-1.870653	-0.577468	-0.892218	N	-2.317342	0.587710	-0.329269
C	-0.514799	-0.742004	-1.303255	Se	-1.888317	3.230775	0.587950
C	-0.116069	-1.971184	-1.886297	I	2.688302	2.885074	-0.616296
C	-1.012715	-2.999627	-2.057416	C	-0.606735	-4.310402	-2.672703
C	0.391650	0.329459	-1.112546	H	0.451211	-4.313429	-2.942056
C	-0.061728	1.490399	-0.534921	H	-0.789091	-5.135157	-1.976559
C	-1.436304	1.512666	-0.181241	H	-1.194084	-4.510392	-3.574404
C	-0.038753	3.692066	0.380889	C	-1.855466	2.741566	2.478666
C	0.670696	2.713461	-0.208445	H	-0.986451	2.109233	2.650564
H	-3.065658	-3.629735	-1.778065	H	-1.800493	3.676552	3.035051
H	-3.812790	-1.496086	-0.755378	H	-2.791640	2.220117	2.675322
H	0.918651	-2.088179	-2.196928				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.195942 hartree
Thermal correction to Gibbs free energy = 0.148709 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12409.9466795 hartree

Entrance2 of the reaction for 7d:

Atom	x	y	z	Atom	x	y	z
C	-2.569125	-2.851816	-2.461863	I	2.391598	2.891678	-1.271530
C	-2.954389	-1.785600	-1.692715	C	-1.723679	2.176914	2.328249
C	-2.056840	-0.712853	-1.476215	H	-0.892398	1.476390	2.293794
C	-0.758648	-0.758310	-2.063499	H	-1.506194	3.049454	2.958229
C	-0.398843	-1.879004	-2.854643	H	-2.655928	1.696925	2.620646
C	-1.277670	-2.916017	-3.059250	C	-0.979373	1.163658	6.253907
C	0.130886	0.319747	-1.835507	C	-0.931949	3.200525	5.388261
C	-0.283686	1.370087	-1.053874	N	-1.172333	1.897187	5.121594
C	-1.605046	1.284555	-0.538076	C	-0.557880	2.043172	7.447643
C	-0.218524	3.429572	0.140825	H	0.408752	1.697045	7.824729
C	0.445092	2.572706	-0.653813	H	-1.284552	1.922618	8.256123
H	-3.259644	-3.674410	-2.626093	C	-0.523860	3.442289	6.851374
H	-3.936757	-1.733257	-1.236230	H	0.463039	3.913356	6.876217
H	0.592559	-1.905065	-3.299017	H	-1.229205	4.140385	7.311383
C	-0.910323	-4.112178	-3.894010	O	-1.017898	4.131694	4.574951
H	1.125737	0.306977	-2.272842	O	-1.114682	-0.053808	6.353409
Br	0.356550	5.012998	0.898219	H	-1.603543	-4.224209	-4.733743
N	-2.467716	0.343843	-0.709763	H	0.102463	-4.023433	-4.292264
Se	-2.010227	2.857474	0.507291	H	-0.968710	-5.029585	-3.299643

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.277079 hartree
Thermal correction to Gibbs free energy = 0.216481 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12770.1256503 hartree

TS2 of the reaction for 7d:

Atom	x	y	z	Atom	x	y	z
C	-2.519031	-2.889653	-2.038144	I	2.372324	2.977773	-1.210865
C	-2.941190	-1.751855	-1.404204	C	-1.703306	2.513291	2.443558
C	-2.054899	-0.656744	-1.251336	H	-0.899084	1.810787	2.268326
C	-0.728361	-0.759127	-1.763268	H	-1.444015	3.494938	2.831237
C	-0.329692	-1.955585	-2.415021	H	-2.669531	2.104963	2.706701
C	-1.197398	-3.010848	-2.557763	C	-1.158225	1.102597	5.543048
C	0.147466	0.339811	-1.602646	C	-0.796194	3.289322	5.238100
C	-0.307124	1.465781	-0.958736	N	-1.200662	2.134230	4.651842
C	-1.654800	1.433472	-0.499880	C	-0.669864	1.585686	6.920217
C	-0.318855	3.636451	-0.000483	H	0.223672	1.020850	7.199548
C	0.397350	2.707074	-0.658816	H	-1.439461	1.369265	7.666198
H	-3.201608	-3.727287	-2.152712	C	-0.418033	3.074263	6.710210
H	-3.946059	-1.656423	-1.007297	H	0.623392	3.372497	6.859212
H	0.683960	-2.023097	-2.801495	H	-1.036476	3.721890	7.337645
C	-0.790021	-4.285545	-3.245253	O	-0.732798	4.384623	4.676853
H	1.163959	0.286923	-1.983727	O	-1.462151	-0.061399	5.309267

Br	0.221542	5.297684	0.611565	H	-1.434126	-4.482167	-4.108390
N	-2.504825	0.467108	-0.618193	H	0.244467	-4.237520	-3.591542
Se	-2.106961	3.087190	0.360696	H	-0.887365	-5.138796	-2.566371

Number of imaginary frequencies = 1 (-443.5229 cm^{-1})
Zero-point vibrational correction = 0.276673 hartree
Thermal correction to Gibbs free energy = 0.216117 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12770.1175757 hartree

Product of the reaction for 7d:

Atom	x	y	z	Atom	x	y	z
C	-2.302969	-2.840429	-1.579294	H	-3.699175	-1.550096	-0.580910
C	-2.694150	-1.681253	-0.968153	H	0.928682	-2.080393	-2.332713
C	-1.779034	-0.603335	-0.822702	H	1.465717	0.231785	-1.550774
C	-0.453348	-0.756315	-1.325525	Br	0.635708	5.334603	0.855377
C	-0.085898	-1.978325	-1.954878	N	-2.202785	0.534120	-0.208239
C	-0.979817	-3.009785	-2.087330	Se	-1.739051	3.153051	0.732503
C	0.448250	0.318073	-1.177772	I	2.733371	2.913364	-0.863115
C	0.021925	1.470987	-0.556666	C	-0.605327	-4.307965	-2.750593
C	-1.331953	1.497338	-0.095537	H	0.434314	-4.297437	-3.085325
C	0.040469	3.647458	0.346157	H	-0.735943	-5.148704	-2.061383
C	0.752854	2.693512	-0.290378	H	-1.243945	-4.499315	-3.619251
H	-3.009411	-3.659533	-1.685973				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.157584 hartree
Thermal correction to Gibbs free energy = 0.113266 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12370.2679141 hartree

Reaction for 7e

Reactant1 of the reaction for 7e:

Atom	x	y	z	Atom	x	y	z
C	-2.282149	-4.081490	-1.454307	H	0.606762	-0.331512	-2.692486
C	-2.391277	-3.076616	-0.521997	N	-1.767864	-0.926783	0.321400
C	-1.638639	-1.881654	-0.644575	Se	-1.420928	1.457951	1.611697
C	-0.763040	-1.721046	-1.748868	H	-1.314060	-4.706524	-3.290499
C	-0.657835	-2.765458	-2.704791	C	-3.072666	-5.356829	-1.336980
C	-1.396568	-3.908855	-2.557198	H	-3.713568	-5.497684	-2.213493
C	-0.051197	-0.507279	-1.846097	H	-2.405085	-6.222938	-1.281611
C	-0.210279	0.469983	-0.885333	H	-3.704489	-5.352065	-0.446234
C	-1.085830	0.183101	0.217559	Br	1.853277	4.360294	-1.314919
C	1.014656	2.787643	-1.161604	C	0.393725	2.045922	2.054390

C	0.451173	1.727540	-1.023721	H	0.400586	2.222130	3.130070
H	-3.053055	-3.172232	0.333716	H	0.653350	2.954595	1.515783
H	0.013120	-2.640338	-3.549873	H	1.095758	1.247963	1.813082

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.194025 hartree
Thermal correction to Gibbs free energy = 0.148778 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -5519.60689274 hartree

Entrance1 of the reaction for 7e:

Atom	x	y	z	Atom	x	y	z
C	0.995359	0.093448	-0.647312	H	3.677441	2.117562	0.047977
C	0.804513	-0.453443	0.599913	H	4.264772	1.936033	2.485945
C	1.639444	-0.096093	1.688311	H	3.893309	-0.976707	6.902425
C	2.683533	0.842548	1.483911	H	4.156370	-1.877927	5.380410
C	2.874603	1.399936	0.191365	H	3.352219	-2.676452	6.752111
C	2.051081	1.031280	-0.838992	N	7.128914	4.434068	2.238053
C	3.475109	1.195766	2.596938	C	6.408585	4.108888	1.093179
N	1.420290	-0.684964	2.900087	C	8.183152	5.325922	2.011256
C	3.222759	0.623009	3.827483	C	7.025481	4.861412	-0.070895
C	2.176213	-0.354317	3.913657	O	5.463223	3.356073	1.066730
C	3.977255	1.054988	4.960072	C	8.190900	5.654035	0.528849
C	4.654069	1.487512	5.862261	O	8.926531	5.732930	2.867217
Br	5.707065	2.167803	7.141648	H	6.255517	5.494626	-0.517323
I	6.690257	3.681409	4.065148	H	7.336852	4.134976	-0.824744
Se	1.720701	-1.209436	5.569472	H	8.084270	6.734850	0.414156
C	3.489348	-1.729699	6.229601	H	9.162657	5.370349	0.118824
H	2.195736	1.457409	-1.828296	H	0.711966	-0.707277	-2.624855
H	0.012622	-1.173634	0.783561	H	-0.645448	-1.000900	-1.522138
C	0.117475	-0.275539	-1.812972	H	-0.384877	0.610173	-2.215653

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.277069 hartree
Thermal correction to Gibbs free energy = 0.213707 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12770.1249273 hartree

TS1 of the reaction for 7e:

Atom	x	y	z	Atom	x	y	z
C	0.047977	-0.916250	-0.093183	H	2.656060	1.376926	-0.699509
C	2.485945	-1.059486	1.265326	H	3.835270	1.953974	1.455399
C	6.902425	-0.331584	1.960641	H	4.681297	-1.246256	5.234179
C	5.380410	0.557985	1.248202	H	3.312273	-2.410454	5.257473
C	6.752111	0.696180	-0.152971	H	4.035839	-1.843802	6.792869
C	2.238053	-0.020818	-0.798117	N	7.183693	4.539901	2.025380
C	1.093179	1.267783	1.973393	C	7.021770	4.739800	0.666187

N	2.011256	-0.510323	3.313048	C	8.257865	5.232654	2.555683
C	-0.070895	1.086151	3.331090	C	8.111788	5.688824	0.182906
C	1.066730	0.158328	3.950969	O	6.152209	4.234927	-0.011338
C	0.528849	1.742216	4.186443	C	8.928953	6.016528	1.433807
C	2.867217	1.671160	5.431465	O	8.593562	5.207892	3.719844
Br	-0.517323	2.079164	6.974857	H	7.637412	6.562932	-0.269273
I	-0.824744	3.288354	3.152298	H	8.690172	5.186604	-0.596092
Se	0.414156	-0.094030	5.857960	H	8.917812	7.077108	1.695756
C	0.118824	-1.573822	5.766415	H	9.973471	5.703592	1.366567
H	-2.624855	0.089450	-1.871148	H	-1.446181	-2.326421	-0.183016
H	-1.522138	-1.731049	1.839939	H	-1.564349	-0.992023	-1.344863
C	-2.215653	-1.678957	-0.848406	H	-0.417161	-2.300114	-1.627254

Number of imaginary frequencies = 1 (-267.0237 cm^{-1})
Zero-point vibrational correction = 0.275496 hartree
Thermal correction to Gibbs free energy = 0.214309 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12770.1057696 hartree

IM of the reaction for 7e:

Atom	x	y	z	Atom	x	y	z
C	-0.109157	-1.125354	-1.125354	H	2.266189	1.136383	1.136383
C	0.190565	-1.188937	-1.188937	H	3.670831	1.848160	1.848160
C	1.245372	-0.419550	-0.419550	H	4.452584	-1.537417	-1.537417
C	2.013549	0.435276	0.435276	H	2.986139	-2.160383	-2.160383
C	1.687170	0.487811	0.487811	H	4.306832	-1.392676	-1.392676
C	0.660238	-0.269094	-0.269094	N	7.350429	4.638106	4.638106
C	3.070982	1.194428	1.194428	C	7.433864	4.847814	4.847814
N	1.495785	-0.515857	-0.515857	C	8.238854	5.420159	5.420159
C	3.327296	1.082966	1.082966	C	8.510165	5.894639	5.894639
C	2.474640	0.202759	0.202759	O	6.754560	4.288959	4.288959
C	4.363392	1.715130	1.715130	C	9.051608	6.283894	6.283894
C	4.306497	1.322561	1.322561	O	8.379673	5.442668	5.442668
Br	5.393593	1.779798	1.779798	H	8.050525	6.723594	6.723594
I	5.792868	3.096795	3.096795	H	9.258774	5.445834	5.445834
S	2.945503	0.206983	0.206983	H	8.900769	7.337291	7.337291
C	3.772403	-1.404627	-1.404627	H	10.114281	6.064791	6.064791
H	0.418875	-0.222024	-0.222024	H	-1.729033	-2.540406	-2.540406
H	-0.372176	-1.827326	-1.827326	H	-1.968058	-1.280307	-1.280307
C	-1.226237	-1.934913	-1.934913	H	-0.843816	-2.601984	-2.601984

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.278588 hartree
Thermal correction to Gibbs free energy = 0.220479 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10766.7718980 hartree

Reactant2 of the reaction for 7e:

Atom	x	y	z	Atom	x	y	z
C	-2.073804	-3.053205	-1.297976	N	-2.084621	0.267615	0.232722
C	-2.428794	-1.978361	-0.515585	Se	-1.781967	2.905595	1.210242
C	-1.687213	-0.776478	-0.561683	I	2.074380	3.450048	-1.497647
C	-0.556198	-0.667679	-1.424505	C	-2.845609	-4.343002	-1.264738
C	-0.208486	-1.785182	-2.227427	H	-3.254955	-4.571177	-2.254021
C	-0.946403	-2.936628	-2.160923	H	-2.191670	-5.174815	-0.984322
C	0.179821	0.539687	-1.446403	H	-3.670686	-4.295280	-0.551594
C	-0.215391	1.574561	-0.632330	H	-0.672604	-3.788152	-2.777277
C	-1.364225	1.330173	0.163427	Br	0.265110	5.394082	1.010147
C	-0.209555	3.698155	0.452527	C	-1.037498	2.334637	2.922886
C	0.387205	2.893248	-0.444533	H	-0.078519	1.857398	2.730776
H	-3.281962	-2.024240	0.153836	H	-0.938295	3.234630	3.529109
H	0.648894	-1.711288	-2.889145	H	-1.762706	1.645099	3.353918
H	1.046139	0.638387	-2.095075				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.196318 hartree
Thermal correction to Gibbs free energy = 0.149726 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12409.9470118 hartree

Entrance2 of the reaction for 7e:

Atom	x	y	z	Atom	x	y	z
C	-2.547069	-2.905000	-2.401550	I	2.380340	2.922760	-1.272757
C	-2.918108	-1.818286	-1.644276	C	-1.722431	2.179673	2.333191
C	-2.028559	-0.737399	-1.445685	H	-0.883205	1.488572	2.299821
C	-0.729915	-0.767080	-2.033703	H	-1.513602	3.056473	2.960083
C	-0.365826	-1.895628	-2.814118	H	-2.648687	1.689978	2.628451
C	-1.249108	-2.927069	-2.988023	C	-0.971032	1.177910	6.258639
C	0.147302	0.321012	-1.818257	C	-0.934628	3.213607	5.389623
C	-0.277446	1.373710	-1.043748	N	-1.170538	1.908882	5.125815
C	-1.596646	1.274663	-0.526272	C	-0.548816	2.060899	7.449487
C	-0.234269	3.440781	0.138839	H	0.420629	1.719341	7.823422
C	0.437635	2.586607	-0.651904	H	-1.271893	1.938490	8.260858
H	-0.962334	-3.788035	-3.585303	C	-0.522797	3.459258	6.851049
H	-3.897500	-1.761681	-1.179685	H	0.462076	3.934676	6.871999
H	0.620924	-1.925698	-3.265904	H	-1.229681	4.154924	7.312340
C	-3.475539	-4.066797	-2.623773	O	-1.027113	4.143142	4.575158
H	1.141206	0.315411	-2.258052	O	-1.101469	-0.039875	6.360587
Br	0.325481	5.033192	0.889287	H	-4.433496	-3.912160	-2.123506
N	-2.449303	0.323272	-0.687204	H	-3.661668	-4.212004	-3.692720
Se	-2.018747	2.850549	0.510006	H	-3.031388	-4.992034	-2.242907

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.277012 hartree

Thermal correction to Gibbs free energy = 0.216210 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12770.1259952 hartree

TS2 of the reaction for 7e:

Atom	x	y	z	Atom	x	y	z
C	-2.526505	-2.914354	-1.945550	I	2.362296	3.017840	-1.276172
C	-2.923336	-1.752704	-1.327161	C	-1.668850	2.530483	2.434275
C	-2.037979	-0.654661	-1.205835	H	-0.818535	1.885853	2.254019
C	-0.715723	-0.750128	-1.730945	H	-1.481565	3.518006	2.847010
C	-0.324002	-1.958196	-2.367763	H	-2.608814	2.054119	2.678170
C	-1.203402	-3.001679	-2.468569	C	-1.012896	1.071351	5.486408
C	0.154377	0.354807	-1.598646	C	-0.883154	3.294784	5.275157
C	-0.300029	1.487953	-0.965665	N	-1.164755	2.129430	4.639539
C	-1.641314	1.450303	-0.490739	C	-0.584614	1.544959	6.886720
C	-0.316016	3.670240	-0.033650	H	0.363087	1.067479	7.150030
C	0.398033	2.738209	-0.690943	H	-1.329695	1.216192	7.616377
H	-0.895719	-3.922573	-2.956106	C	-0.492712	3.059483	6.741013
H	-3.922021	-1.645560	-0.915258	H	0.509624	3.461214	6.913267
H	0.681828	-2.036833	-2.769215	H	-1.181022	3.610063	7.388072
C	-3.451571	-4.092370	-2.082251	O	-0.927566	4.412559	4.758476
H	1.166574	0.302105	-1.991106	O	-1.187104	-0.107751	5.201317
Br	0.218450	5.344656	0.546807	H	-4.430410	-3.882140	-1.646589
N	-2.486682	0.477223	-0.583222	H	-3.590261	-4.353862	-3.136248
Se	-2.094147	3.110359	0.358370	H	-3.032176	-4.971411	-1.582288

Number of imaginary frequencies = 1 (-440.9335 cm^{-1})
Zero-point vibrational correction = 0.276618 hartree
Thermal correction to Gibbs free energy = 0.214615 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12770.1180231 hartree

Product of the reaction for 7e:

Atom	x	y	z	Atom	x	y	z
C	-2.031779	-3.055130	-1.310203	H	0.585134	-1.682019	-3.043242
C	-2.329681	-1.999192	-0.485995	H	1.021072	0.658009	-2.236490
C	-1.592672	-0.786198	-0.547455	N	-1.938065	0.225534	0.295270
C	-0.522668	-0.666638	-1.483250	Se	-1.579732	2.836169	1.300169
C	-0.228935	-1.772635	-2.329673	I	2.033436	3.485879	-1.721066
C	-0.959717	-2.924313	-2.243736	C	-2.805115	-4.344956	-1.256005
C	0.200337	0.541681	-1.533084	H	-3.269929	-4.558807	-2.224120
C	-0.148338	1.566638	-0.681114	H	-2.142255	-5.184817	-1.023059
C	-1.240304	1.323397	0.209785	H	-3.590686	-4.306115	-0.498339
C	-0.147155	3.664021	0.392808	H	-0.728881	-3.763555	-2.894255
C	0.434018	2.886373	-0.545288	Br	0.319766	5.406822	0.846839
H	-3.138004	-2.060215	0.236730				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.157575 hartree
Thermal correction to Gibbs free energy = 0.113226 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12370.2683507 hartree

Reaction for 7f

Reactant1 of the reaction for 7f:

Atom	x	y	z	Atom	x	y	z
C	-2.323238	-2.641830	-1.459501	H	-3.478488	-1.452528	-0.085691
C	-2.557707	-1.558548	-0.649379	H	0.784273	-1.856603	-2.634019
C	-1.581465	-0.538169	-0.528159	H	-0.942823	-3.621023	-2.815629
C	-0.367189	-0.650268	-1.254542	H	1.493369	0.374771	-1.691641
C	-0.148599	-1.780999	-2.082788	Br	3.089255	4.904966	-0.183075
C	-1.108547	-2.756278	-2.181788	N	-1.836181	0.514813	0.301841
C	0.565248	0.403242	-1.127851	Se	-1.477095	2.913359	1.560278
C	0.287433	1.483257	-0.317743	C	0.161238	3.220296	2.587757
C	-0.951079	1.468408	0.414076	H	-0.160039	3.507164	3.589115
C	1.963003	3.516736	-0.241037	H	0.763589	4.006834	2.138772
C	1.190797	2.587469	-0.261091	H	0.728268	2.291088	2.641316
H	-3.072019	-3.421965	-1.550740				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.166163 hartree
Thermal correction to Gibbs free energy = 0.122860 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -5480.29887667 hartree

Entrance1 of the reaction for 7f:

Atom	x	y	z	Atom	x	y	z
C	0.993824	0.148470	-0.654363	H	2.184119	1.522206	-1.835732
C	0.787823	-0.423240	0.576860	H	3.669897	2.154840	0.055183
C	1.625406	-0.078914	1.667206	H	4.255433	1.941949	2.480600
C	2.670085	0.861593	1.468031	H	3.888423	-1.015723	6.868885
C	2.864888	1.437222	0.185337	H	4.148854	-1.901403	5.337194
C	2.040205	1.084454	-0.853357	H	3.345180	-2.713151	6.701265
C	3.465358	1.201251	2.585473	N	7.130804	4.431472	2.255746
N	1.408569	-0.680688	2.873608	C	6.404491	4.119724	1.111066
C	3.215156	0.615722	3.808823	C	8.188574	5.320177	2.032450
C	2.166653	-0.362398	3.888299	C	7.020248	4.879341	-0.048938
C	3.972426	1.034103	4.944803	O	5.455264	3.371805	1.082026
C	4.650874	1.455410	5.850946	C	8.192570	5.660258	0.552740
Br	5.704774	2.119711	7.137644	O	8.936983	5.716417	2.889035
I	6.695356	3.665174	4.077881	H	6.251705	5.520764	-0.486022
Se	1.713742	-1.232352	5.536615	H	7.324232	4.158155	-0.810790

C	3.482961	-1.761141	6.188603	H	8.091986	6.742550	0.447075
H	0.351397	-0.116753	-1.487941	H	9.161042	5.374047	0.136721
H	-0.004967	-1.143456	0.749463				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.249395 hartree
Thermal correction to Gibbs free energy = 0.188603 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12730.8170838 hartree

TS1 of the reaction for 7f:

Atom	x	y	z	Atom	x	y	z
C	0.199954	-0.888396	-0.104638	H	0.911542	0.116950	-1.887957
C	0.342673	-1.050680	1.251544	H	2.661308	1.401834	-0.698803
C	1.336920	-0.324211	1.950041	H	3.831103	1.964650	1.453369
C	2.181643	0.568457	1.238364	H	4.674803	-1.253720	5.221281
C	2.012228	0.716808	-0.161459	H	3.302890	-2.414778	5.238858
C	1.040646	0.002185	-0.816924	H	4.026701	-1.856028	6.777056
C	3.166231	1.276462	1.968661	N	7.184203	4.540492	2.027092
N	1.447568	-0.507272	3.302404	C	7.020314	4.745449	0.668780
C	3.275397	1.089742	3.324353	C	8.261996	5.227537	2.557726
C	2.359869	0.158835	3.942606	C	8.112675	5.692334	0.186755
C	4.233895	1.742459	4.182089	O	6.147693	4.245785	-0.008584
C	4.400737	1.665775	5.426967	C	8.933813	6.012412	1.437061
Br	5.217363	2.069468	6.971660	O	8.599639	5.197581	3.721146
I	5.900088	3.289713	3.151553	H	7.640403	6.569871	-0.260966
Se	2.509267	-0.099301	5.848583	H	8.687497	5.191075	-0.595483
C	3.781053	-1.581405	5.751488	H	8.927740	7.072128	1.702600
H	-0.562690	-1.444424	-0.639882	H	9.976846	5.695279	1.366494
H	-0.289669	-1.725468	1.818602				

Number of imaginary frequencies = 1 (-266.2241 cm^{-1})
Zero-point vibrational correction = 0.247721 hartree
Thermal correction to Gibbs free energy = 0.188823 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12730.7975253 hartree

IM of the reaction for 7f:

Atom	x	y	z	Atom	x	y	z
C	-0.057509	-1.050803	0.033840	H	0.527665	-0.141024	-1.843528
C	0.182192	-1.148956	1.382219	H	2.366390	1.183885	-0.853859
C	1.228831	-0.398605	1.966783	H	3.699397	1.854569	1.158346
C	2.030429	0.455096	1.153427	H	4.524753	-1.504310	4.859289
C	1.755706	0.533013	-0.235782	H	3.148972	-2.301509	5.719374
C	0.734438	-0.204235	-0.780607	H	4.435334	-1.471820	6.661493
C	3.075069	1.198357	1.759142	N	7.294986	4.616790	2.012468
N	1.438930	-0.510339	3.317863	C	7.363599	4.814581	0.662552

C	3.289106	1.077313	3.110889	C	8.205821	5.388426	2.677010
C	2.407185	0.191493	3.792161	C	8.451396	5.842513	0.325233
C	4.310578	1.729481	3.932448	O	6.664660	4.259890	-0.174344
C	4.273170	1.393073	5.228204	C	9.020903	6.229642	1.685986
Br	5.378282	1.946974	6.617091	O	8.363187	5.417667	3.889423
I	5.739356	3.098255	3.058812	H	7.996033	6.676346	-0.215613
Se	2.847905	0.175504	5.679144	H	9.181946	5.379100	-0.343123
C	3.871156	-1.486204	5.729385	H	8.895752	7.287452	1.931850
H	-0.860610	-1.624612	-0.416249	H	10.080744	5.989273	1.804939
H	-0.411419	-1.788680	2.026174				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.249257 hartree
Thermal correction to Gibbs free energy = 0.192029 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12730.8286789 hartree

Reactant2 of the reaction for 7f:

Atom	x	y	z	Atom	x	y	z
C	-2.385691	-2.787083	-1.675392	H	-3.849131	-1.409070	-0.900970
C	-2.810763	-1.588910	-1.156379	H	0.947155	-2.147289	-2.051646
C	-1.878622	-0.548046	-0.943240	H	-0.710126	-3.946466	-2.411310
C	-0.503160	-0.747667	-1.267673	H	1.467734	0.171243	-1.276395
C	-0.098919	-1.996370	-1.804170	Br	0.540158	5.352641	0.982747
C	-1.022302	-2.992030	-2.001678	N	-2.329442	0.640260	-0.428388
C	0.415932	0.305685	-1.038788	Se	-1.891988	3.283778	0.481530
C	-0.043314	1.486281	-0.509076	I	2.735439	2.821102	-0.463982
C	-1.437074	1.546016	-0.244146	C	-2.013048	2.773875	2.363619
C	-0.020981	3.696842	0.386076	H	-1.170076	2.124240	2.591494
C	0.697250	2.696002	-0.153871	H	-1.992058	3.697676	2.940095
H	-3.098315	-3.588129	-1.839559	H	-2.969322	2.262947	2.474310

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.168416 hartree
Thermal correction to Gibbs free energy = 0.123621 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12370.6381072 hartree

Entrance2 of the reaction for 7f:

Atom	x	y	z	Atom	x	y	z
C	-2.526335	-2.877443	-2.442448	Se	-2.005996	2.850136	0.501329
C	-2.915265	-1.806644	-1.676394	I	2.392572	2.921965	-1.285653
C	-2.023697	-0.728089	-1.472385	C	-1.708037	2.171963	2.321879
C	-0.725525	-0.759340	-2.063084	H	-0.870531	1.479017	2.284927
C	-0.356649	-1.879778	-2.850598	H	-1.496131	3.046693	2.950815
C	-1.239188	-2.914200	-3.033767	H	-2.635129	1.683738	2.617025
C	0.154145	0.328789	-1.841489	C	-0.966965	1.157192	6.243747

C	-0.268078	1.376693	-1.061945	C	-0.933221	3.196549	5.383245
C	-1.588218	1.278317	-0.542536	N	-1.148518	1.890443	5.109321
C	-0.220288	3.437850	0.130243	C	-0.580003	2.039873	7.446730
C	0.449887	2.586648	-0.665011	H	0.386317	1.708919	7.837938
H	-3.208239	-3.706333	-2.599260	H	-1.317065	1.904511	8.243301
H	-3.894679	-1.756058	-1.213664	C	-0.559614	3.441239	6.854982
H	0.631171	-1.902505	-3.300240	H	0.417228	3.931084	6.901791
H	-0.953262	-3.770341	-3.635150	H	-1.287718	4.124215	7.302058
H	1.147656	0.323956	-2.282066	O	-1.017268	4.128169	4.570189
Br	0.342580	5.025664	0.887328	O	-1.087030	-0.062228	6.338113
N	-2.441783	0.329682	-0.707655				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.249289 hartree
Thermal correction to Gibbs free energy = 0.190439hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12730.8172322 hartree

TS2 of the reaction for 7f:

Atom	x	y	z	Atom	x	y	z
C	-2.469323	-2.906879	-2.037515	Se	-2.111300	3.078247	0.352124
C	-2.899297	-1.766994	-1.406544	I	2.373706	3.013254	-1.206797
C	-2.019034	-0.668194	-1.256095	C	-1.708667	2.504728	2.433548
C	-0.688290	-0.755727	-1.762842	H	-0.900975	1.805566	2.260777
C	-0.276101	-1.949432	-2.411055	H	-1.453299	3.486584	2.823555
C	-1.148073	-2.999320	-2.543826	H	-2.673327	2.092034	2.695715
C	0.176860	0.352222	-1.601041	C	-1.170564	1.095385	5.538803
C	-0.290407	1.474154	-0.960821	C	-0.800422	3.279952	5.229143
C	-1.640283	1.428054	-0.506544	N	-1.208093	2.124972	4.644992
C	-0.327684	3.645416	-0.004875	C	-0.682172	1.579946	6.915450
C	0.400214	2.722984	-0.660069	H	0.208735	1.012299	7.197455
H	-3.143581	-3.748939	-2.152272	H	-1.453660	1.368417	7.660887
H	-3.904749	-1.673493	-1.010958	C	-0.424322	3.067006	6.702099
H	0.737336	-2.013185	-2.795394	H	0.618164	3.361452	6.851245
H	-0.829322	-3.910240	-3.038985	H	-1.040689	3.718579	7.327482
H	1.194983	0.307647	-1.978907	O	-0.733018	4.373868	4.665555
Br	0.192868	5.313408	0.605255	O	-1.478575	-0.068046	5.307492
N	-2.480519	0.454617	-0.625425				

Number of imaginary frequencies = 1 (-440.8795 cm^{-1})
Zero-point vibrational correction = 0.248925 hartree
Thermal correction to Gibbs free energy = 0.190597 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12730.809866 hartree

Product of the reaction for 7f:

Atom	x	y	z	Atom	x	y	z

C	-2.329682	-2.816425	-1.655050	C	0.770324	2.667429	-0.228824
C	-2.725948	-1.641511	-1.072138	H	-3.044538	-3.621132	-1.792842
C	-1.795573	-0.584068	-0.887969	H	-3.745536	-1.483019	-0.737006
C	-0.445879	-0.762577	-1.316642	H	0.960335	-2.121775	-2.243435
C	-0.068518	-1.994440	-1.919178	H	-0.694742	-3.933863	-2.544174
C	-0.987581	-2.996026	-2.084102	H	1.502296	0.186420	-1.439716
C	0.467759	0.295319	-1.123987	Br	0.640839	5.314862	0.900003
C	0.030964	1.458855	-0.532847	N	-2.229081	0.567647	-0.304617
C	-1.347280	1.513841	-0.149669	Se	-1.767950	3.182956	0.643569
C	0.041361	3.639010	0.360290	I	2.788037	2.839008	-0.675163

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.129788 hartree
Thermal correction to Gibbs free energy = 0.087649 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -12330.9601670 hartree

Reaction for 7g

Reactant1 of the reaction for 7g:

Atom	x	y	z	Atom	x	y	z
C	-2.132385	-2.434273	-1.651187	C	3.977364	6.430308	1.934703
C	-2.556426	-1.196430	-1.244613	H	4.262904	4.358265	1.405293
C	-1.615074	-0.227714	-0.813543	H	0.237628	5.810723	1.118370
C	-0.236268	-0.563468	-0.812290	C	3.060031	7.471844	2.069567
C	0.169063	-1.854662	-1.239274	H	5.025805	6.597559	2.159753
C	-0.752065	-2.785913	-1.654939	H	3.396256	8.449714	2.399436
C	0.676702	0.426627	-0.384768	N	-2.072992	0.992583	-0.403802
C	0.212508	1.662352	0.010170	Se	-1.907545	3.599464	0.536502
C	-1.209818	1.888067	-0.011769	C	1.711330	7.260010	1.780386
C	1.688599	3.697508	0.787159	H	0.997297	8.070833	1.883776
C	1.075400	2.718135	0.423398	C	-0.340621	-4.159939	-2.111814
H	-2.858650	-3.173128	-1.980131	H	-0.656411	-4.336440	-3.145195
H	-3.607120	-0.925200	-1.239280	H	0.742607	-4.288691	-2.057560
H	1.229241	-2.096832	-1.233294	H	-0.810014	-4.931841	-1.493304
H	1.742466	0.216046	-0.378440	C	-1.556771	3.401643	2.443981
C	2.202592	4.959798	1.221549	H	-1.982976	4.283716	2.923134
C	3.555487	5.174105	1.511949	H	-0.482998	3.359181	2.627481
C	1.279506	6.010041	1.356659	H	-2.058608	2.506574	2.808085

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.285348 hartree
Thermal correction to Gibbs free energy = 0.236068 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -3189.18405768 hartree

Entrance1 of the reaction for 7g:

Atom	x	y	z	Atom	x	y	z
C	-2.345281	-3.060905	-0.098411	C	1.508103	2.055119	-0.222702
C	-1.058505	-2.886967	0.339213	C	2.090131	3.121737	-0.254380
C	-0.406255	-1.641748	0.151207	C	2.847039	4.336951	-0.279343
C	-1.110332	-0.589979	-0.489771	C	2.433772	5.422490	-1.065714
C	-2.441352	-0.803798	-0.933298	C	4.016373	4.436382	0.490123
C	-3.062783	-2.015127	-0.747927	C	3.188454	6.589010	-1.084005
H	-2.840122	-4.017525	0.047837	H	1.524894	5.340525	-1.653201
H	-0.509202	-3.682791	0.831260	C	4.765241	5.607096	0.462730
N	0.882923	-1.505387	0.574825	H	4.319657	3.596563	1.107929
C	-0.441432	0.644618	-0.633025	C	4.353698	6.682972	-0.322938
H	-2.965847	0.013573	-1.422116	H	2.867031	7.427472	-1.692939
C	0.848924	0.790908	-0.166081	H	5.669015	5.681262	1.058392
C	1.487084	-0.358662	0.416570	H	4.939559	7.596187	-0.340342
H	-0.954183	1.488682	-1.086176	I	-0.732040	4.161569	0.802549
Se	3.284289	-0.275072	1.088120	I	-2.932054	5.485954	1.660244
C	4.208978	0.459563	-0.474828	C	-4.473802	-2.262979	-1.209608
H	4.258934	1.545701	-0.430512	H	-5.115041	-2.541174	-0.366914
H	5.211493	0.031566	-0.464802	H	-4.897845	-1.375666	-1.684796
H	3.688002	0.139255	-1.377047	H	-4.507950	-3.087650	-1.929019

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.286119 hartree
Thermal correction to Gibbs free energy = 0.223395 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16970.1682965 hartree

TS1 of the reaction for 7g:

Atom	x	y	z	Atom	x	y	z
C	0.001575	0.064742	-0.066130	C	1.207284	0.004713	-2.289169
C	-0.030887	0.077893	1.303792	H	3.362169	-0.051185	-0.601070
C	1.179232	0.044045	2.040703	H	4.561103	-0.060959	1.599157
C	2.411132	-0.002700	1.339711	H	3.184057	-2.223333	5.751626
C	2.409673	-0.015404	-0.078341	H	1.404680	-2.380631	5.917953
C	1.230733	0.017387	-0.784520	H	2.414602	-2.026388	7.351501
C	3.599955	-0.030365	2.103627	C	5.902076	-1.303522	7.377923
N	1.117499	0.054584	3.404872	C	5.602264	1.104475	7.656546
C	3.535649	-0.012432	3.476058	C	6.464231	-1.373217	8.644609
C	2.228562	0.022535	4.083191	C	6.591003	-0.215625	9.413888
C	4.697922	-0.025775	4.342242	C	6.160796	1.019501	8.922373
C	4.901666	0.004706	5.583418	H	5.801524	-2.190658	6.760993
C	5.472307	-0.059924	6.877604	H	5.257103	2.052448	7.258029
I	6.863182	-0.138136	3.376470	H	6.804307	-2.326486	9.033808
I	9.368804	-0.298117	1.824473	H	7.029130	-0.275140	10.404859
Se	2.094461	0.055998	6.004892	H	6.264182	1.912173	9.529179
C	2.296807	-1.871538	6.278620	H	0.703837	0.896376	-2.676465

H	-0.928344	0.091093	-0.627961	H	2.217965	-0.025732	-2.701817
H	-0.965143	0.113838	1.853995	H	0.657231	-0.865807	-2.660978

Number of imaginary frequencies = 1 (-145.7234 cm^{-1})
Zero-point vibrational correction = 0.285707 hartree
Thermal correction to Gibbs free energy = 0.227022 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16970.1564038 hartree

IM of the reaction for 7g:

Atom	x	y	z	Atom	x	y	z
C	-2.296858	-2.704067	-1.986694	H	1.553465	4.205111	2.507804
C	-2.729360	-1.441793	-1.676215	H	-0.651236	6.154658	-0.631856
C	-1.797970	-0.461663	-1.257051	C	1.080895	7.523437	1.947682
C	-0.417407	-0.803563	-1.162876	H	2.145748	6.411171	3.454192
C	-0.009990	-2.120978	-1.495059	H	1.337972	8.490902	2.366135
C	-0.921870	-3.066190	-1.900967	N	-2.253058	0.794086	-0.957821
C	0.503994	0.184556	-0.737523	Se	-1.803907	3.454176	-0.107221
C	0.041137	1.439814	-0.421624	I	2.871631	2.480764	0.282908
C	-1.357676	1.635476	-0.569001	C	0.288360	7.447301	0.803699
C	0.069265	3.718293	0.315645	H	-0.070465	8.352644	0.325952
C	0.783911	2.606210	0.058969	C	-0.505465	-4.467344	-2.255966
H	-3.013298	-3.455009	-2.308239	H	-0.775113	-4.699257	-3.291285
H	-3.775278	-1.162214	-1.741609	H	0.571889	-4.602770	-2.141976
H	1.044762	-2.372232	-1.421547	H	-1.014899	-5.195231	-1.616457
H	1.561065	-0.054417	-0.659697	C	-2.461013	3.148938	1.706153
C	0.426670	5.031985	0.867086	H	-3.460999	2.727848	1.611058
C	1.210411	5.114162	2.025579	H	-1.772873	2.465939	2.201260
C	-0.043790	6.208249	0.267830	H	-2.488559	4.123250	2.193197
C	1.537775	6.356446	2.557504	I	6.290868	2.140376	0.622691

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288162 hartree
Thermal correction to Gibbs free energy = 0.230850 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16970.1901807 hartree

Reactant2 of the reaction for 7g:

Atom	x	y	z	Atom	x	y	z
C	-2.306115	-2.712751	-1.972242	H	1.479857	4.183533	2.546082
C	-2.737822	-1.451250	-1.657581	H	-0.582422	6.161217	-0.673977
C	-1.803231	-0.469925	-1.249857	C	1.094437	7.507927	1.954317
C	-0.420234	-0.809409	-1.172052	H	2.083553	6.383847	3.503099
C	-0.014088	-2.125939	-1.508106	H	1.355259	8.472081	2.377873
C	-0.929584	-3.072756	-1.902433	N	-2.256787	0.784730	-0.945137
C	0.503886	0.180666	-0.758419	Se	-1.807084	3.447087	-0.101482
C	0.039468	1.433511	-0.437358	I	2.835967	2.519498	0.230136

C	-1.360452	1.628171	-0.566328	C	0.338827	7.443088	0.784757
C	0.061339	3.720047	0.307921	H	0.013403	8.353411	0.293081
C	0.771328	2.608648	0.035049	C	-0.516406	-4.473574	-2.261088
H	-3.024689	-3.465220	-2.285001	H	-0.800236	-4.706643	-3.292272
H	-3.784842	-1.173708	-1.710836	H	0.562380	-4.608259	-2.161313
H	1.041711	-2.375934	-1.447022	H	-1.017264	-5.200584	-1.613956
H	1.562099	-0.057356	-0.693808	C	-2.455120	3.150779	1.716939
C	0.428792	5.028281	0.863151	H	-3.456191	2.731721	1.623350
C	1.174913	5.097671	2.047017	H	-1.768388	2.467448	2.213288
C	-0.001272	6.208887	0.243013	H	-2.480508	4.127971	2.198220
C	1.507783	6.335649	2.585113				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288106 hartree
Thermal correction to Gibbs free energy = 0.237428 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10079.5244134 hartree

Entrance2 of the reaction for 7g:

Atom	x	y	z	Atom	x	y	z
C	-2.298576	-2.701619	-2.021066	H	1.420557	4.191458	2.569871
C	-2.728327	-1.436338	-1.719900	H	-0.540291	6.153572	-0.720889
C	-1.797658	-0.460431	-1.289209	C	1.089930	7.512967	1.930417
C	-0.420310	-0.810452	-1.174922	H	2.024997	6.395666	3.517284
C	-0.015570	-2.131006	-1.498093	H	1.349213	8.479024	2.350710
C	-0.927042	-3.071809	-1.914287	N	-2.250936	0.796910	-0.997331
C	0.499714	0.173768	-0.739707	Se	-1.807952	3.452185	-0.130795
C	0.035855	1.430234	-0.433084	I	2.824565	2.501466	0.291409
C	-1.359753	1.636942	-0.595922	C	0.362703	7.442992	0.743295
C	0.054447	3.718637	0.299979	H	0.057909	8.351229	0.234660
C	0.764212	2.601912	0.050405	C	-0.514741	-4.477102	-2.257249
H	-3.014857	-3.449478	-2.349902	H	-0.775094	-4.713643	-3.293889
H	-3.771714	-1.151211	-1.798920	H	0.560554	-4.618180	-2.130868
H	1.036312	-2.388890	-1.407784	H	-1.035115	-5.198084	-1.618778
H	1.554187	-0.071502	-0.646893	C	-2.469930	3.142599	1.702084
C	0.423710	5.028355	0.850923	H	-3.480462	2.750767	1.606322
C	1.141631	5.103140	2.051536	H	-1.799316	2.436077	2.185218
C	0.022073	6.206325	0.207465	H	-2.467354	4.110709	2.199357
C	1.474315	6.343542	2.584258	I	-3.575105	2.649579	4.909221

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288086 hartree
Thermal correction to Gibbs free energy = 0.230098 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16970.1908115 hartree

TS2 of the reaction for 7g:

Atom	x	y	z	Atom	x	y	z
C	-2.305382	-2.673285	-2.070175	H	1.341168	4.217912	2.591995
C	-2.729827	-1.403867	-1.783508	H	-0.500370	6.147942	-0.781440
C	-1.804700	-0.433723	-1.321008	C	1.074017	7.533008	1.891636
C	-0.436567	-0.801450	-1.160149	H	1.948480	6.428737	3.521534
C	-0.036232	-2.128550	-1.469831	H	1.335537	8.502353	2.303107
C	-0.941344	-3.059110	-1.917327	N	-2.257114	0.824370	-1.046269
C	0.476505	0.171733	-0.694046	Se	-1.815084	3.471114	-0.170760
C	0.016820	1.436098	-0.408093	I	2.793308	2.481917	0.400312
C	-1.372700	1.669230	-0.618887	C	0.379852	7.452229	0.685646
C	0.024603	3.724386	0.291187	H	0.102146	8.355901	0.153558
C	0.740560	2.598491	0.088815	C	-0.532814	-4.468845	-2.248163
H	-3.018556	-3.413183	-2.423431	H	-0.759649	-4.702384	-3.293433
H	-3.766879	-1.107316	-1.898389	H	0.536239	-4.621313	-2.085732
H	1.009478	-2.397379	-1.343841	H	-1.081280	-5.186008	-1.629005
H	1.524394	-0.084771	-0.562780	C	-2.476597	3.046313	1.987060
C	0.403261	5.037679	0.832819	H	-3.457286	2.661133	1.747160
C	1.088211	5.124555	2.051604	H	-1.679353	2.350240	2.208688
C	0.037429	6.210954	0.160688	H	-2.390851	4.065581	2.336984
C	1.422920	6.369025	2.574388	I	-3.245560	2.530601	4.644009

Number of imaginary frequencies = 1 (-448.6740 cm^{-1})
Zero-point vibrational correction = 0.287061 hartree
Thermal correction to Gibbs free energy = 0.229907 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16970.1837906 hartree

Product of the reaction for 7g:

Atom	x	y	z	Atom	x	y	z
C	-2.310403	-2.692291	-2.013743	C	-0.047464	6.169493	0.254576
C	-2.748247	-1.444097	-1.666558	C	1.525968	6.375829	2.543386
C	-1.827580	-0.461634	-1.209776	H	1.457883	4.225398	2.601163
C	-0.446165	-0.804908	-1.122678	H	-0.658479	6.086237	-0.639882
C	-0.031311	-2.114784	-1.493264	C	1.117713	7.527754	1.873045
C	-0.931335	-3.051680	-1.931908	H	2.128052	6.453011	3.442895
C	0.461359	0.174597	-0.669323	H	1.408197	8.504987	2.244970
C	-0.012689	1.421405	-0.324409	N	-2.299307	0.768990	-0.873622
C	-1.420321	1.639453	-0.458028	Se	-1.880564	3.398505	0.059723
C	-0.037974	3.683875	0.415281	I	2.783386	2.517558	0.327693
C	0.706330	2.583016	0.156334	C	0.329426	7.421903	0.728852
H	-3.021746	-3.436843	-2.361767	H	0.006036	8.314949	0.204139
H	-3.795999	-1.168714	-1.727862	C	-0.506432	-4.440431	-2.327490
H	1.025322	-2.361860	-1.421422	H	-0.766700	-4.644613	-3.371337
H	1.520408	-0.058958	-0.594228	H	0.571392	-4.574085	-2.210900
C	0.373358	5.007745	0.913472	H	-1.014038	-5.192395	-1.714403
C	1.155867	5.121698	2.069111				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.249447 hartree
Thermal correction to Gibbs free energy = 0.201414 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10039.8417118 hartree

Reaction for 7h

Reactant1 of the reaction for 7h:

Atom	x	y	z	Atom	x	y	z
C	-1.631200	-2.822328	-1.075219	H	0.063430	5.694350	1.430924
C	-1.775644	-1.838834	-0.125114	C	2.516502	7.764544	-0.744250
C	-1.144549	-0.579075	-0.275172	H	2.686468	5.983276	-1.949882
C	-0.350833	-0.328018	-1.424695	C	1.926298	8.348824	0.375966
C	-0.208427	-1.351756	-2.398156	H	0.582582	8.067639	2.038278
C	-0.831170	-2.558806	-2.223977	H	3.202341	8.339119	-1.358510
C	0.253125	0.942267	-1.543442	H	2.153404	9.378874	0.631882
C	0.059745	1.887344	-0.559018	N	-1.316625	0.354772	0.708711
C	-0.746413	1.520184	0.576204	Se	-1.042405	2.804629	1.983330
C	1.003893	4.343606	-0.561939	C	-2.295567	-4.165195	-0.931176
C	0.607675	3.200628	-0.626733	H	-2.971981	-4.355117	-1.770969
H	-2.375838	-2.000307	0.765639	H	-1.551129	-4.968082	-0.927154
H	0.398434	-1.160098	-3.278632	H	-2.871771	-4.226025	-0.005476
H	0.858585	1.176706	-2.414475	H	-0.719581	-3.338875	-2.972547
C	1.345265	5.705296	-0.287315	C	0.759988	2.768548	2.725317
C	0.750269	6.295339	0.840202	H	0.734939	3.404274	3.611029
C	2.230625	6.445425	-1.080351	H	1.473700	3.163933	2.002378
C	1.043502	7.612711	1.167304	H	1.007711	1.747785	3.012119

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.285343 hartree
Thermal correction to Gibbs free energy = 0.236041 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -3189.18436254 hartree

Entrance1 of the reaction for 7h:

Atom	x	y	z	Atom	x	y	z
C	-2.361321	-3.083986	-0.073419	C	2.088675	3.121619	-0.263684
C	-1.066474	-2.884946	0.344838	C	2.849708	4.334339	-0.285977
C	-0.419396	-1.639470	0.148532	C	2.438657	5.424619	-1.066963
C	-1.121545	-0.581804	-0.485586	C	4.021004	4.426721	0.481427
C	-2.457136	-0.799793	-0.915326	C	3.197207	6.588706	-1.081738
C	-3.053723	-2.015434	-0.713332	H	1.528279	5.348376	-1.652904
H	-0.504438	-3.675469	0.833285	C	4.773872	5.594942	0.457365
N	0.874789	-1.505311	0.560728	H	4.322611	3.583416	1.095333
C	-0.452824	0.650684	-0.633133	C	4.364366	6.675585	-0.322778

H	-2.993211	0.011053	-1.399977	H	5.679102	5.663458	1.051498
C	0.842128	0.793795	-0.176554	H	4.953217	7.586919	-0.337470
C	1.480025	-0.359706	0.398038	H	-4.076287	-2.178931	-1.042514
H	-0.968227	1.496128	-1.080721	I	-0.723074	4.167208	0.806065
Se	3.283621	-0.285174	1.053529	I	-2.919803	5.492986	1.670724
C	4.196518	0.466769	-0.508104	C	-3.063085	-4.400197	0.126430
H	4.260427	1.551220	-0.444941	H	-2.417047	-5.122887	0.629297
H	5.193575	0.026315	-0.519629	H	-3.968029	-4.268908	0.728653
H	3.659413	0.169611	-1.408795	H	-3.372397	-4.824124	-0.834550
C	1.503764	2.056442	-0.233345	H	2.877271	7.430841	-1.686382

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.286039 hartree
Thermal correction to Gibbs free energy = 0.223215 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16970.1685977 hartree

TS1 of the reaction for 7h:

Atom	x	y	z	Atom	x	y	z
C	0.001698	0.040266	-0.059960	H	1.280340	-0.017535	-1.808537
C	-0.029066	0.055175	1.315069	H	3.393774	-0.068174	-0.533894
C	1.169105	0.025820	2.069281	H	4.561911	-0.069421	1.700365
C	2.418428	-0.018588	1.398926	H	3.105607	-2.231087	5.819622
C	2.437610	-0.034094	-0.020001	H	1.323622	-2.395136	5.947242
C	1.262152	-0.005651	-0.722178	H	2.301007	-2.039647	7.402888
C	3.590664	-0.041012	2.185323	C	5.783058	-1.301760	7.509802
N	1.080507	0.038081	3.433237	C	5.469866	1.105371	7.780580
C	3.498085	-0.021005	3.556720	C	6.317208	-1.369266	8.788661
C	2.177833	0.010385	4.133605	C	6.423404	-0.210989	9.560019
C	4.641118	-0.029056	4.447664	C	6.000480	1.022624	9.058506
C	4.818098	0.002565	5.693079	H	5.698854	-2.189484	6.891297
C	5.360603	-0.059717	6.999419	H	5.130727	2.052135	7.374101
I	6.826119	-0.130257	3.529508	H	6.651435	-2.321345	9.185750
I	9.367308	-0.278326	2.032476	H	6.839536	-0.268794	10.560529
Se	2.002451	0.043711	6.052642	H	6.087682	1.915838	9.667049
C	2.205898	-1.883482	6.327956	H	-2.146466	0.108222	-0.242895
C	-1.259942	0.070931	-0.879316	H	-1.271353	0.944563	-1.539106
H	-0.968915	0.089526	1.857804	H	-1.329089	-0.816957	-1.516159

Number of imaginary frequencies = 1 (-145.6156 cm^{-1})
Zero-point vibrational correction = 0.285640 hartree
Thermal correction to Gibbs free energy = 0.226586 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16970.1567595 hartree

IM of the reaction for 7h:

Atom	x	y	z	Atom	x	y	z

C	-1.915842	-3.108070	-1.190139	C	1.871646	6.756031	1.346507
C	-2.134912	-2.095299	-0.285645	H	2.314094	4.778326	0.622341
C	-1.516320	-0.833930	-0.448029	C	0.873270	7.651059	1.726930
C	-0.652974	-0.601709	-1.558428	H	-1.245840	7.958987	1.966756
C	-0.441068	-1.658409	-2.482784	H	2.915149	7.047630	1.399074
C	-1.054231	-2.868635	-2.299049	H	1.138071	8.645343	2.071143
C	-0.038273	0.664277	-1.700521	N	-1.773684	0.144298	0.476533
C	-0.285962	1.637250	-0.760415	Se	-1.417860	2.765864	1.476601
C	-1.171803	1.267404	0.285206	I	1.523927	3.708656	-2.184410
C	-0.157259	3.742265	0.375061	C	-2.562952	-4.457078	-1.037919
C	0.240871	2.999792	-0.675783	H	-3.181816	-4.687885	-1.910940
H	-2.785718	-2.235479	0.571882	H	-1.803669	-5.242043	-0.961844
H	0.213182	-1.488844	-3.332443	H	-3.193012	-4.498289	-0.147233
H	0.622898	0.858151	-2.540767	H	-0.886079	-3.672041	-3.010734
C	0.192685	5.093819	0.831678	C	-0.202115	2.212863	2.901085
C	-0.805856	5.992109	1.231521	H	-0.713546	1.430111	3.459956
C	1.537283	5.480687	0.904912	H	0.715626	1.854996	2.437925
C	-0.465188	7.266409	1.670829	H	-0.029678	3.091843	3.521558
H	-1.851809	5.701730	1.177804	I	3.618857	4.783625	-4.712626

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288149 hartree
Thermal correction to Gibbs free energy = 0.230826 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16970.1905221 hartree

Reactant2 of the reaction for 7h:

Atom	x	y	z	Atom	x	y	z
C	-1.915018	-3.115390	-1.183768	C	1.881119	6.738955	1.359297
C	-2.129293	-2.102607	-0.277678	H	2.317164	4.751262	0.659127
C	-1.515749	-0.840342	-0.446845	C	0.884471	7.645429	1.716915
C	-0.662357	-0.606353	-1.565553	H	-1.234975	7.975682	1.921850
C	-0.455748	-1.662648	-2.491279	H	2.926169	7.020559	1.430784
C	-1.064049	-2.874177	-2.300608	H	1.153077	8.638736	2.060754
C	-0.052497	0.660692	-1.713565	N	-1.767567	0.138197	0.478803
C	-0.295205	1.631019	-0.770101	Se	-1.414283	2.761377	1.475444
C	-1.170367	1.261946	0.283627	I	1.468968	3.717940	-2.171695
C	-0.162780	3.741390	0.376693	C	-2.556053	-4.466139	-1.025293
C	0.221056	2.995775	-0.677682	H	-3.177883	-4.700658	-1.895140
H	-2.771955	-2.243861	0.585640	H	-1.792798	-5.247469	-0.951875
H	0.190114	-1.492655	-3.347192	H	-3.181302	-4.508195	-0.131449
H	0.600175	0.854856	-2.560326	H	-0.900228	-3.677813	-3.012918
C	0.194353	5.092071	0.826927	C	-0.198170	2.216676	2.903003
C	-0.803352	6.000277	1.205757	H	-0.716062	1.441117	3.466132
C	1.541953	5.464474	0.919399	H	0.717523	1.849637	2.443403
C	-0.456898	7.274015	1.641572	H	-0.024302	3.100367	3.516376
H	-1.850607	5.717843	1.140025				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288071 hartree
Thermal correction to Gibbs free energy = 0.237445 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10079.5247248 hartree

Entrance2 of the reaction for 7h:

Atom	x	y	z	Atom	x	y	z
C	-1.928663	-3.107624	-1.192869	C	1.865082	6.742110	1.364972
C	-2.150737	-2.090650	-0.293894	H	2.306433	4.747065	0.688536
C	-1.530016	-0.830797	-0.458891	C	0.865435	7.654207	1.698810
C	-0.661573	-0.604758	-1.567098	H	-1.256125	7.991874	1.866789
C	-0.447344	-1.665433	-2.486362	H	2.909741	7.019707	1.455521
C	-1.062666	-2.873922	-2.299778	H	1.131405	8.648406	2.042272
C	-0.044648	0.659241	-1.710994	N	-1.789064	0.150200	0.461308
C	-0.295468	1.632951	-0.773451	Se	-1.425505	2.767761	1.464904
C	-1.184932	1.272498	0.272382	I	1.487784	3.712996	-2.162691
C	-0.172463	3.744151	0.368955	C	-2.575195	-4.456155	-1.035515
C	0.222801	2.996014	-0.679198	H	-3.184327	-4.696139	-1.912900
H	-2.803209	-2.226759	0.562879	H	-1.814907	-5.238500	-0.944076
H	0.211297	-1.501022	-3.333685	H	-3.213891	-4.490541	-0.150803
H	0.620542	0.847848	-2.549249	H	-0.891977	-3.681033	-3.006641
C	0.182707	5.097148	0.814364	C	-0.195437	2.203358	2.899676
C	-0.818357	6.010634	1.170117	H	-0.696881	1.398515	3.433400
C	1.529487	5.465829	0.927339	H	0.730585	1.872795	2.435351
C	-0.475630	7.286465	1.602831	H	-0.046024	3.068893	3.542341
H	-1.864792	5.728528	1.090974	I	1.861599	1.160848	5.449685

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.288053 hartree
Thermal correction to Gibbs free energy = 0.229967 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16970.1909493 hartree

TS2 of the reaction for 7h:

Atom	x	y	z	Atom	x	y	z
C	-1.973255	-3.094446	-3.094446	C	1.798853	6.733036	1.456330
C	-2.211674	-2.072457	-2.072457	H	2.260533	4.720848	0.845238
C	-1.560330	-0.821638	-0.821638	C	0.789907	7.661061	1.708091
C	-0.642354	-0.617541	-0.617541	H	-1.334253	8.021385	1.732739
C	-0.408958	-1.686262	-1.686262	H	2.838713	7.002971	1.607004
C	-1.054679	-2.881553	-2.881553	H	1.043927	8.659836	2.047614
C	-0.000540	0.634018	0.634018	N	-1.839243	0.159822	0.457561
C	-0.278340	1.617982	1.617982	Se	-1.470083	2.768615	1.468558
C	-1.216716	1.284275	1.284275	I	1.576253	3.674912	-2.058358
C	-0.206965	3.729547	3.729547	C	-2.655177	-4.428940	-1.072141

C	0.244301	2.973606	2.973606	H	-3.232490	-4.656582	-1.974104
H	-2.903784	-2.194319	-2.194319	H	-1.917571	-5.228578	-0.948977
H	0.288921	-1.535617	-1.535617	H	-3.331531	-4.448841	-0.215204
H	0.702664	0.809394	0.809394	H	-0.870184	-3.693483	-2.969014
C	0.137473	5.091423	5.091423	C	0.093208	2.118662	3.019729
C	-0.873544	6.021423	6.021423	H	-0.504229	1.352794	3.493846
C	1.477616	5.451297	5.451297	H	0.841711	1.827680	2.295939
C	-0.545909	7.303289	7.303289	H	0.185252	3.079818	3.506247
H	-1.914552	5.743097	5.743097	I	2.062092	1.336178	4.874048

Number of imaginary frequencies = 1 (-445.9436 cm^{-1})
Zero-point vibrational correction = 0.286900 hartree
Thermal correction to Gibbs free energy = 0.229676 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16970.1841966 hartree

Product of the reaction for 7h:

Atom	x	y	z	Atom	x	y	z
C	5.762667	-0.318745	0.018768	C	-4.917227	-1.825332	-0.860296
C	4.700900	-1.187678	0.038194	H	-2.931463	-2.228661	-1.586519
C	3.360877	-0.714769	0.032972	C	-5.071146	-0.273983	0.980235
C	3.117537	0.690678	0.006407	H	-3.206232	0.521354	1.701576
C	4.232134	1.576026	-0.012576	C	-5.689024	-1.120579	0.061301
C	5.507830	1.085756	-0.006298	H	-5.391825	-2.487972	-1.576614
C	1.784344	1.146537	-0.000407	H	-5.666085	0.266635	1.709187
C	0.760135	0.224503	0.022456	H	-6.768177	-1.235024	0.067544
C	1.134525	-1.155794	0.047474	N	2.351598	-1.627293	0.052530
C	-1.440794	-0.682482	0.041474	Se	-0.394893	-2.266271	0.076959
C	-0.672934	0.432192	0.014549	I	-1.440373	2.365540	-0.126701
H	4.854107	-2.262753	0.057692	C	7.186226	-0.806937	0.022698
H	4.047725	2.646456	-0.032171	H	7.718643	-0.456337	-0.867647
H	1.574721	2.213204	-0.022769	H	7.725821	-0.422238	0.894415
C	-2.907453	-0.821245	0.044149	H	7.232352	-1.897902	0.043500
C	-3.533286	-1.682914	-0.865206	H	6.352499	1.769273	-0.020871
C	-3.688171	-0.124463	0.974688				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.249440 hartree
Thermal correction to Gibbs free energy = 0.201473 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10039.8423839 hartree

Reaction for 7i

Reactant1 of the reaction for 7i:

Atom	x	y	z	Atom	x	y	z
C	-2.114019	-3.129746	0.138276	H	4.988391	0.598297	-1.197417
C	-0.783915	-2.865707	0.352187	H	3.601713	-0.329206	-1.825049
C	-0.291842	-1.543592	0.221286	C	1.274714	2.320386	-0.074947
C	-1.187435	-0.499214	-0.131790	C	1.904983	3.354816	-0.086268
C	-2.556984	-0.799884	-0.347955	C	2.831321	4.443326	-0.030180
C	-3.008528	-2.088683	-0.215118	C	2.496664	5.751246	-0.401576
H	-2.488948	-4.143154	0.238956	C	4.129680	4.149957	0.418601
H	-0.080325	-3.646371	0.622005	C	3.456701	6.754786	-0.323855
N	1.041702	-1.322207	0.430992	H	1.491741	5.970338	-0.747287
C	-0.659965	0.807548	-0.243478	C	5.080677	5.159231	0.491363
H	-3.235020	0.004957	-0.617376	H	4.354141	3.125140	0.703805
C	0.679569	1.027579	-0.012841	C	4.745630	6.462258	0.120635
C	1.502686	-0.108431	0.318674	H	3.198463	7.769016	-0.611094
H	-1.314021	1.636284	-0.499363	H	6.083348	4.931704	0.838963
Se	3.385390	0.149109	0.645283	H	5.489649	7.250334	0.179267
C	3.901427	0.510275	-1.199726	H	-4.056282	-2.317432	-0.380341
H	3.452079	1.442754	-1.541756				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.257587 hartree
Thermal correction to Gibbs free energy = 0.210599 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -3149.87622538 hartree

Entrance1 of the reaction for 7i:

Atom	x	y	z	Atom	x	y	z
C	-2.355000	-3.066328	-0.048442	H	3.684020	0.086969	-1.396761
C	-1.061764	-2.886519	0.376019	C	1.500495	2.057080	-0.217793
C	-0.416962	-1.640282	0.178014	C	2.083844	3.122853	-0.254740
C	-1.123988	-0.585629	-0.457512	C	2.843056	4.336733	-0.282878
C	-2.458942	-0.798371	-0.888275	C	2.425146	5.426764	-1.060387
C	-3.060136	-2.015042	-0.687109	C	4.020011	4.429404	0.475802
H	-2.846851	-4.021626	0.103179	C	3.182686	6.591318	-1.080780
H	-0.502758	-3.677971	0.863911	H	1.510395	5.350127	-1.639318
N	0.877802	-1.502657	0.589219	C	4.771620	5.598322	0.446543
C	-0.455061	0.648807	-0.607993	H	4.327080	3.585980	1.086718
H	-2.990781	0.015359	-1.372562	C	4.355322	6.678843	-0.330375
C	0.839160	0.794267	-0.154289	H	2.857716	7.433304	-1.682939
C	1.480864	-0.357319	0.423620	H	5.681173	5.667508	1.033938
H	-0.972481	1.492070	-1.056827	H	4.943297	7.590662	-0.349321
Se	3.284566	-0.274404	1.077476	H	-4.081110	-2.178418	-1.015510
C	4.194726	0.441995	-0.501871	I	-0.735206	4.163165	0.811773
H	4.220929	1.529620	-0.484227	I	-2.937806	5.483501	1.668574
H	5.206315	0.036445	-0.477928				

Number of imaginary frequencies = 0

Zero-point vibrational correction = 0.258346 hartree
Thermal correction to Gibbs free energy = 0.197770 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16930.8602821 hartree

TS1 of the reaction for 7i:

Atom	x	y	z	Atom	x	y	z
C	-1.884021	-3.213366	0.086213	H	3.395948	0.063505	-2.189271
C	-0.578886	-2.790897	0.144086	C	0.751900	2.672789	0.068098
C	-0.282714	-1.406386	0.114544	C	1.859280	3.266244	0.139072
C	-1.342796	-0.466739	0.025597	C	2.899686	4.226232	0.117435
C	-2.681652	-0.930007	-0.033446	C	3.293892	4.786357	-1.112325
C	-2.943859	-2.276702	-0.003584	C	3.536455	4.610283	1.311882
H	-2.111738	-4.273978	0.108998	C	4.312087	5.728630	-1.138862
H	0.248502	-3.489037	0.212523	H	2.787429	4.483971	-2.023231
N	1.027239	-1.018376	0.169903	C	4.555406	5.549154	1.270130
C	-1.006496	0.906554	0.004657	H	3.225150	4.161195	2.248896
H	-3.486660	-0.204445	-0.101447	C	4.940975	6.106611	0.048412
C	0.309936	1.292189	0.068281	H	4.616599	6.169804	-2.081426
C	1.306984	0.252057	0.142474	H	5.051494	5.850499	2.186047
H	-1.795192	1.650654	-0.056433	H	5.738321	6.842222	0.022460
Se	3.165664	0.751647	0.238522	H	-3.967826	-2.632073	-0.048445
C	3.421257	1.026676	-1.682550	I	-0.859090	4.406290	-0.098362
H	2.640644	1.686027	-2.062978	I	-3.131942	6.276050	-0.325406
H	4.398052	1.495186	-1.805969				

Number of imaginary frequencies = 1 (-145.9241 cm^{-1})
Zero-point vibrational correction = 0.257970 hartree
Thermal correction to Gibbs free energy = 0.201481 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16930.8481348 hartree

IM of the reaction for 7i:

Atom	x	y	z	Atom	x	y	z
C	-1.906726	-3.114556	0.086156	H	3.891659	-0.267712	-1.286928
C	-0.620948	-2.666672	0.261378	C	0.769437	2.782590	-0.102117
C	-0.339474	-1.283845	0.166275	C	2.096690	2.901647	0.092777
C	-1.392223	-0.362416	-0.112041	C	3.016384	4.046294	0.049471
C	-2.709496	-0.859100	-0.286080	C	2.966624	4.946623	-1.022843
C	-2.957931	-2.204966	-0.189027	C	3.972957	4.227112	1.057775
H	-2.125068	-4.174607	0.159289	C	3.845793	6.022912	-1.069175
H	0.199454	-3.343170	0.474559	H	2.245878	4.795095	-1.819076
N	0.951950	-0.864380	0.353861	C	4.847946	5.306186	1.006495
C	-1.089007	1.018493	-0.207135	H	4.017993	3.536245	1.895724
H	-3.509949	-0.156770	-0.496615	C	4.784784	6.206384	-0.055681
C	0.209948	1.431624	-0.034153	H	3.800255	6.715236	-1.903010
C	1.150072	0.403159	0.244014	H	5.577164	5.444339	1.797550

H	-1.877812	1.735566	-0.417484	H	5.469301	7.047216	-0.095737
Se	2.899805	1.180637	0.482509	H	-3.966520	-2.580762	-0.322990
C	3.633966	0.790673	-1.284697	I	-0.512796	4.413793	-0.450543
H	2.872234	1.029818	-2.024539	I	-2.707758	7.014898	-1.012858
H	4.521330	1.412798	-1.398151				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.260153 hartree
Thermal correction to Gibbs free energy = 0.204287 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16930.8818351 hartree

Reactant2 of the reaction for 7i:

Atom	x	y	z	Atom	x	y	z
C	-1.896005	-3.135940	0.079656	H	4.509964	1.453020	-1.412283
C	-0.609843	-2.685935	0.247153	H	3.937613	-0.247918	-1.295903
C	-0.333579	-1.302145	0.157212	C	0.774553	2.759391	-0.091248
C	-1.391597	-0.381843	-0.108211	C	2.102526	2.887334	0.094535
C	-2.708741	-0.880868	-0.274380	C	3.012962	4.038071	0.051866
C	-2.952008	-2.228008	-0.182183	C	2.982950	4.915872	-1.039721
H	-2.110984	-4.196842	0.148874	C	3.942865	4.241668	1.080390
H	0.213855	-3.361327	0.450288	C	3.856826	5.996257	-1.085393
N	0.957611	-0.879561	0.337912	H	2.286492	4.741286	-1.853130
C	-1.093092	1.000062	-0.197690	C	4.811013	5.326114	1.029574
H	-3.513189	-0.180352	-0.475033	H	3.972830	3.564981	1.930228
C	0.206405	1.412873	-0.032158	C	4.768221	6.204823	-0.051642
C	1.152844	0.387834	0.233154	H	3.830963	6.670582	-1.934616
H	-1.886652	1.715166	-0.397100	H	5.520483	5.484157	1.834511
Se	2.902249	1.168638	0.471016	H	5.449402	7.048268	-0.091606
C	3.644125	0.801037	-1.298295	H	-3.960398	-2.606332	-0.309775
H	2.873664	1.010991	-2.037708	I	-0.478632	4.381919	-0.414205

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.260195 hartree
Thermal correction to Gibbs free energy = 0.211716 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10040.2158571 hartree

Entrance2 of the reaction for 7i:

Atom	x	y	z	Atom	x	y	z
C	-3.678503	-5.023127	1.404559	H	2.366574	-2.464779	0.597834
C	-2.426898	-4.565364	1.733381	C	-0.799001	0.746698	0.845324
C	-2.087727	-3.213208	1.493975	C	0.483040	0.881843	1.234879
C	-3.048261	-2.333219	0.912212	C	1.428229	2.003282	1.168722
C	-4.332944	-2.838782	0.586241	C	1.622268	2.684847	-0.039594
C	-4.637983	-4.154356	0.827410	C	2.170420	2.369370	2.299214
H	-3.939967	-6.060154	1.585788	C	2.529554	3.736376	-0.104412

H	-1.675929	-5.211155	2.174886	H	1.075485	2.377861	-0.925120
N	-0.832499	-2.783837	1.836028	C	3.072037	3.425035	2.228381
C	-2.687388	-0.984154	0.675783	H	2.027837	1.839895	3.237392
H	-5.062358	-2.168468	0.142366	C	3.251187	4.110397	1.027893
C	-1.421198	-0.566439	1.005038	H	2.680004	4.256654	-1.044183
C	-0.571347	-1.548914	1.581310	H	3.635661	3.710226	3.110118
H	-3.406630	-0.298991	0.235014	H	3.959825	4.930099	0.972620
Se	1.144906	-0.769000	1.984825	H	-5.620553	-4.538014	0.574853
C	2.143260	-1.416266	0.410584	I	-1.913485	2.320951	0.076166
H	1.514594	-1.281199	-0.466070	I	3.817471	-2.457971	-2.397381
H	3.053375	-0.821822	0.354748				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.260338 hartree
Thermal correction to Gibbs free energy = 0.204872 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16930.8824644 hartree

TS2 of the reaction for 7i:

Atom	x	y	z	Atom	x	y	z
C	-1.883930	-3.127852	0.156497	H	3.827459	-0.301445	-1.434738
C	-0.606988	-2.670999	0.361431	C	0.800798	2.749588	-0.112593
C	-0.319473	-1.289633	0.231609	C	2.122248	2.868548	0.135592
C	-1.365637	-0.382763	-0.113870	C	3.022227	4.030528	0.099483
C	-2.676464	-0.889405	-0.318396	C	3.042661	4.872792	-1.019521
C	-2.927717	-2.230395	-0.185929	C	3.899266	4.275112	1.164075
H	-2.102759	-4.185798	0.255817	C	3.912453	5.957278	-1.058288
H	0.206669	-3.338581	0.623451	H	2.389579	4.665524	-1.861078
N	0.962650	-0.867973	0.446544	C	4.762805	5.364127	1.121889
C	-1.060242	0.991972	-0.242896	H	3.890813	3.621015	2.031811
H	-3.469321	-0.195726	-0.581282	C	4.769602	6.207280	0.011984
C	0.232459	1.410635	-0.034981	H	3.926505	6.601779	-1.930816
C	1.177745	0.401307	0.310034	H	5.431243	5.552589	1.955246
H	-1.841825	1.699842	-0.506014	H	5.447704	7.053648	-0.022224
Se	2.905824	1.173932	0.557600	H	-3.930262	-2.613349	-0.343674
C	3.655057	0.756689	-1.570934	I	-0.435043	4.369235	-0.527536
H	2.752386	1.079931	-2.071030	I	4.551844	0.246873	-4.192111
H	4.501602	1.428379	-1.538314				

Number of imaginary frequencies = 1 (-446.7444 cm^{-1})
Zero-point vibrational correction = 0.259213 hartree
Thermal correction to Gibbs free energy = 0.204129 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -16930.8755875 hartree

Product of the reaction for 7i:

Atom	x	y	z	Atom	x	y	z

C	-1.892046	-3.132060	0.204036	C	0.853098	2.702235	-0.189603
C	-0.611283	-2.683861	0.394209	C	2.179151	2.800370	0.064774
C	-0.301812	-1.306974	0.230440	C	3.061464	3.980096	0.052211
C	-1.341546	-0.399563	-0.133935	C	3.086996	4.840008	-1.052817
C	-2.659955	-0.898559	-0.323962	C	3.913663	4.231766	1.134667
C	-2.928420	-2.231176	-0.159094	C	3.936457	5.941498	-1.063575
H	-2.122286	-4.184940	0.330841	H	2.451791	4.632771	-1.907863
H	0.195217	-3.354512	0.671544	C	4.757767	5.337578	1.122493
N	0.982943	-0.902071	0.429358	H	3.900352	3.565602	1.992791
C	-1.020303	0.965250	-0.292516	C	4.770138	6.195307	0.024302
H	-3.445112	-0.201136	-0.601548	H	3.952076	6.598210	-1.927321
C	0.278751	1.376130	-0.095382	H	5.406186	5.528094	1.971421
C	1.228838	0.368588	0.268627	H	5.431599	7.055569	0.013383
H	-1.794555	1.676895	-0.568123	H	-3.935861	-2.606371	-0.305180
Se	2.948866	1.118901	0.495639	I	-0.375246	4.334197	-0.607305

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.221619 hartree
Thermal correction to Gibbs free energy = 0.175800 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10000.5340897 hartree

Reaction for 7j

Reactant1 of the reaction for 7j:

Atom	x	y	z	Atom	x	y	z
C	-1.811697	-4.162014	-1.977859	C	0.569317	5.366171	0.625048
C	-2.269239	-3.464848	-0.890627	C	0.995619	6.714520	0.834631
C	-1.812238	-2.144637	-0.649537	C	0.483718	7.458247	1.909326
C	-0.881052	-1.566040	-1.550538	C	1.929417	7.300336	-0.034456
C	-0.426754	-2.315602	-2.666670	C	0.903256	8.768065	2.107544
C	-0.875792	-3.594845	-2.890122	C	-0.238110	7.000684	2.577745
C	-0.455569	-0.245686	-1.288239	H	2.342147	8.610804	0.172812
C	-0.945201	0.429464	-0.188623	C	2.321606	6.720798	-0.863646
C	-1.864721	-0.263242	0.672381	H	1.831315	9.346016	1.241919
C	-0.193763	2.924572	0.238222	C	0.505026	9.339682	2.939546
C	-0.555417	1.777357	0.065187	H	3.064130	9.059834	-0.501483
H	-2.165189	-5.174062	-2.157743	H	2.156313	10.369305	1.400367
H	-2.980997	-3.894779	-0.193508	H	-2.276803	-1.480836	0.449567
H	0.286244	-1.856978	-3.347698	N	-2.586327	0.633287	2.206708
C	-0.406884	-4.406680	-4.067673	Se	-0.938831	0.730997	3.249532
H	0.302556	-3.845531	-4.679753	C	-1.203391	1.229126	4.182587
H	0.080608	-5.328564	-3.734217	H	-0.188381	1.316020	2.719039
H	-1.252097	-4.697349	-4.699944	H	-0.586453	-0.278144	3.454940
H	0.245246	0.242431	-1.959683	H	0.569317	5.366171	0.625048

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.296934 hartree
Thermal correction to Gibbs free energy = 0.242796 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -3265.33179740 hartree

Entrance1 of the reaction for 7j:

Atom	x	y	z	Atom	x	y	z
C	-0.005137	-0.013698	-0.023175	H	4.581984	0.097107	1.578932
C	-0.014605	-0.031338	1.347067	H	2.690929	-2.505974	5.805475
C	1.207423	-0.019362	2.065913	H	4.174628	-1.567048	6.183054
C	2.427305	0.013685	1.341828	H	2.965550	-1.890091	7.454170
C	2.402408	0.030358	-0.076941	C	8.047619	0.426764	6.148923
C	1.212104	0.016985	-0.763233	C	9.275237	0.534283	6.871567
C	3.624117	0.045329	2.088595	C	10.500598	0.463352	6.190368
N	1.166101	-0.055346	3.429515	C	9.260019	0.710729	8.264057
C	3.575341	0.035525	3.468355	C	11.692115	0.567493	6.897550
C	2.285559	-0.038911	4.100279	C	11.673141	0.742824	8.280993
C	4.779155	0.136277	4.224686	C	10.457679	0.814409	8.961026
C	5.827589	0.232989	4.836951	H	10.505123	0.327513	5.114033
C	7.004658	0.335893	5.532364	H	8.309609	0.765696	8.784079
I	4.478029	3.217170	5.247256	H	12.637695	0.512083	6.368398
I	3.998496	5.854394	5.605173	H	12.606028	0.824198	8.829334
Se	2.132547	-0.040577	6.016551	H	10.442923	0.951484	10.037139
C	3.113635	-1.691572	6.392160	C	1.162539	0.034530	-2.267363
H	-0.945018	-0.023837	-0.568863	H	0.613475	0.910582	-2.627451
H	-0.940132	-0.056887	1.912468	H	2.166227	0.058050	-2.697406
H	3.346611	0.056302	-0.615274	H	0.645484	-0.851806	-2.649093

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.297567 hartree
Thermal correction to Gibbs free energy = 0.230252 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3124654 hartree

TS1 of the reaction for 7j:

Atom	x	y	z	Atom	x	y	z
C	0.033908	-0.018273	-0.046021	H	3.395017	-0.031780	-0.585622
C	0.001892	0.003440	1.324101	H	4.596411	-0.044207	1.610086
C	1.212744	0.013555	2.059299	H	1.239651	-2.240415	5.989389
C	2.445771	-0.000811	1.356176	H	0.014025	-1.029446	5.475859
C	2.442330	-0.021230	-0.062171	H	0.427208	-1.212231	7.212488
C	1.262424	-0.029898	-0.766980	C	5.893972	-0.465676	7.961957
C	3.636355	-0.010637	2.116519	C	6.468560	-0.587754	9.252606
N	1.157108	0.053306	3.422420	C	6.708049	-1.862404	9.796956
C	3.574959	-0.003925	3.490885	C	6.796762	0.567556	9.984736
C	2.270192	0.047219	4.093297	C	7.269885	-1.973208	11.060917

C	4.727561	-0.095254	4.361077	C	7.593452	-0.824418	11.784545
C	4.846141	-0.233973	5.623467	C	7.357382	0.442211	11.247842
C	5.410587	-0.357167	6.844641	H	6.451513	-2.745041	9.221301
I	6.852935	-0.040679	3.440240	H	6.608314	1.544244	9.552472
I	9.424256	0.063106	1.912310	H	7.457083	-2.954095	11.483998
S	2.163483	0.120974	6.008601	H	8.032956	-0.916735	12.772371
C	0.801836	-1.264622	6.191283	H	7.612320	1.330418	11.815483
H	-0.897404	-0.025532	-0.606165	H	0.712070	0.826047	-2.662995
H	-0.932904	0.015733	1.874394	H	2.247489	-0.059824	-2.685380
C	1.236883	-0.051362	-2.271510	H	0.707396	-0.936759	-2.637912

Number of imaginary frequencies = 1 (-156.4669 cm^{-1})
Zero-point vibrational correction = 0.296284 hartree
Thermal correction to Gibbs free energy = 0.234028 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.2980294 hartree

IM of the reaction for 7j:

Atom	x	y	z	Atom	x	y	z
C	-2.370899	-4.208137	-1.658121	C	0.131962	8.289600	2.520300
C	-2.742608	-3.157605	-0.860525	H	-1.128287	6.543994	2.624388
C	-2.011176	-1.947419	-0.904842	C	1.972680	8.172094	0.956239
C	-0.892146	-1.837399	-1.781834	H	2.144765	6.332318	-0.157401
C	-0.541258	-2.947096	-2.592478	C	1.247118	8.873324	1.919348
C	-1.258162	-4.119195	-2.542557	H	-0.431608	8.836056	3.269170
C	-0.165196	-0.622508	-1.812335	H	2.839828	8.626617	0.489003
C	-0.558493	0.412265	-0.996184	H	1.551021	9.875980	2.201849
C	-1.695400	0.160391	-0.181719	N	-2.406259	-0.909685	-0.102524
C	-0.551829	2.552324	0.068419	Se	-2.101881	1.725645	0.878725
C	0.036353	1.731347	-0.834007	I	1.723565	2.325558	-1.918285
H	-2.933998	-5.136650	-1.622197	C	-0.897781	-5.304560	-3.395625
H	-3.590525	-3.221492	-0.187291	H	-0.027454	-5.094743	-4.020557
H	0.311914	-2.854184	-3.259064	H	-0.673157	-6.175172	-2.771229
H	0.693210	-0.514304	-2.470081	H	-1.733325	-5.578695	-4.047552
C	-0.214632	3.854813	0.461704	C	-1.298184	1.133933	2.557435
C	0.078055	4.978403	0.815584	H	-0.329906	0.692733	2.328036
C	0.466355	6.298703	1.194277	H	-1.206036	2.016649	3.189259
C	-0.262203	7.006235	2.162646	H	-1.987592	0.409581	2.990187
C	1.588656	6.888123	0.590456	I	4.515979	3.278888	-3.695604

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298502 hartree
Thermal correction to Gibbs free energy = 0.236721 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17406.3346026 hartree

Reactant2 of the reaction for 7j:

Atom	x	y	z	Atom	x	y	z
C	-2.377631	-4.208294	-1.646075	C	0.060714	0.060714	2.454915
C	-2.741357	-3.154279	-0.849362	H	-1.229235	-1.229235	2.477480
C	-2.005004	-1.947838	-0.901164	C	2.030147	2.030147	1.060452
C	-0.889962	-1.844560	-1.785112	H	2.272386	2.272386	-0.001839
C	-0.547737	-2.957555	-2.594569	C	1.232623	1.232623	1.944009
C	-1.269193	-4.126640	-2.536818	H	-0.558477	-0.558477	3.141097
C	-0.158760	-0.632934	-1.822984	H	2.940863	2.940863	0.663856
C	-0.544014	0.403563	-1.005485	H	1.524727	1.524727	2.234610
C	-1.676161	0.159906	-0.183336	N	-2.390428	-2.390428	-0.099515
C	-0.528024	2.552449	0.065116	Se	-2.072964	-2.072964	0.877924
C	0.045534	1.723504	-0.840386	I	1.699320	1.699320	-1.928331
H	-2.944026	-5.134447	-1.604395	C	-0.918600	-0.918600	-3.387433
H	-3.585777	-3.212971	-0.171452	H	-0.050787	-0.050787	-4.017947
H	0.302011	-2.870577	-3.266215	H	-0.695012	-0.695012	-2.760613
H	0.695030	-0.531191	-2.487716	H	-1.759313	-1.759313	-4.033212
C	-0.183164	3.851905	0.453714	C	-1.263958	-1.263958	2.555445
C	0.106710	4.975749	0.810329	H	-0.301077	-0.301077	2.324470
C	0.482255	6.295936	1.198513	H	-1.163983	-1.163983	3.182462
C	-0.319107	7.029712	2.086797	H	-1.959898	-1.959898	2.991756
C	1.661250	6.859390	0.684793				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298326 hartree
Thermal correction to Gibbs free energy = 0.242366 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10155.6674832 hartree

Entrance2 of the reaction for 7j:

Atom	x	y	z	Atom	x	y	z
C	-2.388373	-4.196009	-1.671400	C	0.144240	8.255240	2.549104
C	-2.758561	-3.133443	-0.889553	H	-1.079140	6.482860	2.643014
C	-2.010622	-1.933238	-0.933612	C	1.959680	8.203176	0.951565
C	-0.876396	-1.846652	-1.793972	H	2.148349	6.387703	-0.197841
C	-0.527951	-2.968302	-2.589333	C	1.237169	8.871613	1.940012
C	-1.261048	-4.130058	-2.539598	H	-0.415502	8.775935	3.318730
C	-0.133292	-0.642373	-1.823397	H	2.810015	8.683628	0.479429
C	-0.526698	0.402570	-1.020897	H	1.526928	9.874275	2.236872
C	-1.679325	0.177156	-0.220774	N	-2.404442	-0.884028	-0.147433
C	-0.516595	2.555902	0.036305	Se	-2.082750	1.750578	0.822389
C	0.071185	1.717533	-0.850904	I	1.754440	2.283050	-1.906659
H	-2.963355	-5.117127	-1.634601	C	-0.902969	-5.328801	-3.374652
H	-3.616216	-3.180087	-0.227460	H	-0.024237	-5.134816	-3.992996
H	0.337222	-2.893666	-3.242672	H	-0.692630	-6.193418	-2.737125
H	0.736421	-0.553383	-2.469017	H	-1.734379	-5.603630	-4.031532
C	-0.167267	3.855170	0.423906	C	-1.312797	1.163790	2.540283
C	0.121241	4.977672	0.785158	H	-0.349767	0.701117	2.337124

C	0.493731	6.297096	1.179972	H	-1.219894	2.053312	3.159860
C	-0.231782	6.971510	2.174122	H	-2.023950	0.460205	2.968600
C	1.594007	6.919135	0.568641	I	-0.260661	0.153931	5.647663

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298415 hartree
Thermal correction to Gibbs free energy = 0.235876 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3331539 hartree

TS2 of the reaction for 7j:

Atom	x	y	z	Atom	x	y	z
C	-2.424870	-4.161925	-1.678572	C	0.065346	8.342081	2.435380
C	-2.808418	-3.095354	-0.910403	H	-1.234201	6.622544	2.470529
C	-2.051818	-1.897179	-0.932787	C	2.018840	8.161099	1.022051
C	-0.893485	-1.822958	-1.761873	H	2.238442	6.298162	-0.043062
C	-0.530067	-2.951287	-2.544332	C	1.235491	8.893461	1.913988
C	-1.271183	-4.106933	-2.514184	H	-0.542995	8.912171	3.129520
C	-0.142584	-0.626027	-1.771780	H	2.929285	8.590409	0.617404
C	-0.553826	0.426017	-0.985252	H	1.537619	9.894646	2.203532
C	-1.733110	0.219468	-0.212228	N	-2.460549	-0.849486	-0.157482
C	-0.579820	2.573666	0.061121	Se	-2.142336	1.773792	0.822698
C	0.043436	1.734596	-0.805139	I	1.760621	2.292981	-1.814421
H	-3.008187	-5.078476	-1.657156	C	-0.897513	-5.311028	-3.335279
H	-3.685563	-3.134547	-0.273541	H	0.000976	-5.125060	-3.927411
H	0.354604	-2.883758	-3.172252	H	-0.712292	-6.176157	-2.690486
H	0.747812	-0.545211	-2.389967	H	-1.710095	-5.582024	-4.017003
C	-0.225008	3.877695	0.440435	C	-1.155375	0.971988	2.727506
C	0.072821	5.001355	0.788811	H	-0.208354	0.721851	2.269515
C	0.459988	6.320939	1.172474	H	-1.228443	1.878340	3.311180
C	-0.326286	7.060183	2.069333	H	-1.874505	0.183410	2.902827
C	1.637157	6.878590	0.648941	I	0.072479	-0.046902	5.054683

Number of imaginary frequencies = 1 (-446.0539 cm^{-1})
Zero-point vibrational correction = 0.297440 hartree
Thermal correction to Gibbs free energy = 0.235706 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3264277 hartree

Product of the reaction for 7j:

Atom	x	y	z	Atom	x	y	z
C	-2.311891	-4.214560	-1.694716	C	-0.169730	6.948499	2.194482
C	-2.648931	-3.187290	-0.857026	C	1.571514	6.904127	0.503273
C	-1.920147	-1.967507	-0.888557	C	0.199507	8.245046	2.532113
C	-0.835462	-1.840031	-1.806734	H	-0.984794	6.452760	2.711105
C	-0.517685	-2.932333	-2.662038	C	1.932584	8.200745	0.848412
C	-1.230822	-4.102754	-2.620188	H	2.096263	6.371473	-0.283170

C	-0.115815	-0.628380	-1.830198	C	1.248858	8.872714	1.861549
C	-0.482437	0.386297	-0.971730	H	-0.332625	8.767370	3.320335
C	-1.590446	0.134105	-0.100543	H	2.748976	8.688634	0.326175
C	-0.498204	2.488932	0.133146	H	1.533744	9.885287	2.128266
C	0.089321	1.699572	-0.806206	N	-2.285467	-0.967771	-0.041010
H	-2.875007	-5.143697	-1.663094	Se	-1.952869	1.630440	0.999662
H	-3.470399	-3.270197	-0.153062	I	1.711518	2.338180	-1.930434
H	0.310734	-2.820243	-3.357505	C	-0.906029	-5.265983	-3.518490
H	0.716634	-0.501011	-2.517956	H	-0.061369	-5.038759	-4.172719
C	-0.144039	3.802941	0.495180	H	-0.654935	-6.154152	-2.929356
C	0.146145	4.935270	0.819682	H	-1.765730	-5.525486	-4.145000
C	0.515805	6.268914	1.175920				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.259832 hartree
Thermal correction to Gibbs free energy = 0.207178 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10115.9865730 hartree

Reaction for 7k

Reactant1 of the reaction for 7k:

Atom	x	y	z	Atom	x	y	z
C	-1.814333	-4.151852	-2.001241	C	0.212016	4.251382	0.448386
C	-2.261884	-3.432184	-0.918185	C	0.569963	5.397758	0.633675
C	-1.801773	-2.114101	-0.677384	C	0.995142	6.745702	0.848212
C	-0.865925	-1.527727	-1.569005	C	0.504588	7.475643	1.942109
C	-0.410861	-2.280637	-2.683544	C	1.906884	7.344898	-0.035096
C	-0.873873	-3.552680	-2.888171	C	0.923330	8.784978	2.145218
C	-0.441086	-0.209875	-1.301479	H	-0.200203	7.007852	2.621549
C	-0.935388	0.461997	-0.201276	C	2.318981	8.654770	0.177175
C	-1.858590	-0.235741	0.651143	H	2.282666	6.776060	-0.879138
C	-0.189040	2.956374	0.237389	C	1.829454	9.376213	1.265422
C	-0.547147	1.808746	0.059284	H	0.541676	9.345825	2.992166
C	-2.291633	-5.553306	-2.271224	H	3.023866	9.114097	-0.508202
H	-3.007838	-5.881732	-1.515143	H	2.153943	10.399052	1.427770
H	-2.772861	-5.616124	-3.252677	N	-2.270708	-1.452260	0.422455
H	-1.450590	-6.254355	-2.277518	Se	-2.587173	0.652957	2.187229
H	-2.977232	-3.853989	-0.218198	C	-0.942301	0.753555	3.233920
H	0.304808	-1.831038	-3.366010	H	-1.213537	1.237310	4.172580
H	-0.523354	-4.126067	-3.742238	H	-0.196206	1.351933	2.712388
H	0.262982	0.279910	-1.968334	H	-0.581233	-0.254822	3.427691

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.296908 hartree
Thermal correction to Gibbs free energy = 0.242926 hartree

M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -3265.33208075 hartree

Entrance1 of the reaction for 7k:

Atom	x	y	z	Atom	x	y	z
C	-0.060480	0.011313	-0.052583	H	4.562053	0.038837	1.549356
C	-0.040338	-0.012664	1.322451	H	4.316043	-0.956726	6.810225
C	1.184796	-0.029332	2.034055	H	3.551166	-2.110256	5.677161
C	2.407941	-0.017670	1.313862	H	2.940498	-1.970892	7.342841
C	2.374815	0.004990	-0.105551	C	8.009689	0.376754	6.152128
C	1.174519	0.018699	-0.763729	C	9.227554	0.480798	6.891508
C	3.603777	-0.005401	2.059114	C	10.453184	0.588010	6.215467
N	1.146103	-0.075811	3.397315	C	9.202732	0.476436	8.294986
C	3.557879	-0.016956	3.439844	C	11.635378	0.689036	6.938535
C	2.266257	-0.082213	4.068706	C	11.606857	0.684620	8.332851
C	4.761583	0.089115	4.193045	C	10.391091	0.578527	9.007902
C	5.806657	0.189614	4.810733	H	10.465113	0.591230	5.130720
C	6.975778	0.290143	5.519661	H	8.252235	0.393751	8.811266
I	4.518182	3.179334	5.175218	H	12.581093	0.771949	6.413292
I	4.044354	5.815423	5.555349	H	12.532423	0.764264	8.893698
Se	2.062183	-0.081706	5.974034	H	10.368915	0.575484	10.092616
C	3.382046	-1.425971	6.508571	C	-1.353012	0.028735	-0.822837
H	-0.960454	-0.022376	1.898982	H	-2.215232	0.022213	-0.152759
H	1.151661	0.036773	-1.849900	H	-1.414279	0.920263	-1.455466
H	3.312068	0.014089	-0.654327	H	-1.421997	-0.842156	-1.482868

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.297681 hartree
Thermal correction to Gibbs free energy = 0.230936 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3134287 hartree

TS1 of the reaction for 7k:

Atom	x	y	z	Atom	x	y	z
C	0.036230	-0.021824	-0.038643	H	3.428361	-0.051348	-0.519122
C	0.006848	0.005069	1.336603	H	4.600178	-0.059856	1.709668
C	1.206031	0.012857	2.088397	H	1.118125	-2.213786	6.026613
C	2.456108	-0.008911	1.415105	H	-0.076201	-0.984056	5.484423
C	2.472404	-0.034730	-0.004036	H	0.299153	-1.167412	7.229924
C	1.295720	-0.040943	-0.704202	C	5.756925	-0.478484	8.092226
C	3.630506	-0.020889	2.197109	C	6.299952	-0.604134	9.396083
N	1.124658	0.057818	3.451221	C	6.535196	-1.880361	9.938663
C	3.541640	-0.009498	3.570582	C	6.600121	0.548955	10.143602
C	2.224517	0.049372	4.143346	C	7.065030	-1.994927	11.216026
C	4.674473	-0.103851	4.465386	C	7.360374	-0.848323	11.955020
C	4.762455	-0.242436	5.731017	C	7.128382	0.419872	11.420207
C	5.299860	-0.367642	6.964022	H	6.300474	-2.761211	9.351090

I	6.816302	-0.055339	3.591726	H	6.415280	1.526896	9.712614
I	9.425459	0.039555	2.121597	H	7.248947	-2.977021	11.637742
Se	2.080790	0.131776	6.055940	H	7.774448	-0.943575	12.953498
C	0.692819	-1.230088	6.216508	H	7.361248	1.306330	11.999929
C	-1.227439	-0.029663	-0.855045	H	-2.113494	-0.012559	-0.217160
H	-0.933132	0.023833	1.879854	H	-1.263114	0.839635	-1.519692
H	1.311785	-0.060883	-1.790358	H	-1.273533	-0.922567	-1.486947

Number of imaginary frequencies = 1 (-158.1035 cm^{-1})
Zero-point vibrational correction = 0.296257 hartree
Thermal correction to Gibbs free energy = 0.233851 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.2984299 hartree

IM of the reaction for 7k:

Atom	x	y	z	Atom	x	y	z
C	-2.381791	-4.229883	-1.623596	H	-1.135864	6.551469	2.627745
C	-2.732442	-3.158480	-0.834685	C	1.946715	8.193649	0.939578
C	-1.999838	-1.951021	-0.888194	H	2.123753	6.352293	-0.170629
C	-0.882130	-1.833592	-1.766374	C	1.222126	8.892976	1.904798
C	-0.536621	-2.949271	-2.573601	H	-0.449262	8.849050	3.263467
C	-1.265656	-4.105883	-2.499752	H	2.808731	8.652090	0.466700
C	-0.158599	-0.619224	-1.801591	H	1.521583	9.898085	2.183306
C	-0.552867	0.416847	-0.986015	N	-2.394994	-0.910880	-0.086251
C	-1.686911	0.160460	-0.170061	Se	-2.096522	1.726418	0.890417
C	-0.551464	2.558063	0.076312	I	1.719347	2.336547	-1.916236
C	0.037281	1.737720	-0.826578	H	-0.994094	-4.954974	-3.120579
H	-3.577159	-3.210815	-0.154877	C	-3.147206	-5.523689	-1.583782
H	0.311953	-2.867880	-3.245815	H	-3.557086	-5.758637	-2.571304
H	0.697945	-0.510406	-2.461711	H	-2.489472	-6.351569	-1.300245
C	-0.218718	3.862805	0.465968	H	-3.971667	-5.476817	-0.869651
C	0.069791	4.988666	0.816029	C	-1.288214	1.134639	2.566870
C	0.452624	6.311999	1.189835	H	-0.318172	0.698314	2.335563
C	-0.274917	7.017624	2.160359	H	-1.199411	2.016303	3.200589
C	1.568295	6.906579	0.578839	H	-1.973994	0.406204	2.998582
C	0.113597	8.304127	2.512938	I	4.502398	3.298648	-3.705175

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298482 hartree
Thermal correction to Gibbs free energy = 0.236662 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3351967 hartree

Reactant2 of the reaction for 7k:

Atom	x	y	z	Atom	x	y	z
C	-2.390542	-4.230835	-1.613387	H	-1.238348	6.593144	2.480352
C	-2.732687	-3.156030	-0.824858	C	2.002497	8.166695	1.039213

C	-1.994425	-1.953048	-0.884698	H	2.250646	6.303199	-0.018298
C	-0.879991	-1.842425	-1.769035	C	1.205424	8.891952	1.924927
C	-0.543339	-2.961249	-2.575437	H	-0.578710	8.894276	3.132409
C	-1.277670	-4.114000	-2.494920	H	2.908033	8.607055	0.635808
C	-0.151677	-0.631799	-1.810795	H	1.492589	9.898626	2.210347
C	-0.538032	0.406099	-0.993966	N	-2.379864	-0.909216	-0.083172
C	-1.667926	0.158070	-0.171003	Se	-2.067969	1.726210	0.890257
C	-0.527781	2.556348	0.073944	I	1.696579	2.319100	-1.923480
C	0.046824	1.727683	-0.831397	H	-1.013008	-4.965874	-3.114796
H	-3.574248	-3.202736	-0.140930	C	-3.162037	-5.520405	-1.567952
H	0.302296	-2.886205	-3.252029	H	-3.581648	-5.751464	-2.552262
H	0.700675	-0.529709	-2.477359	H	-2.505553	-6.351697	-1.291878
C	-0.187639	3.858317	0.458386	H	-3.979717	-5.470306	-0.846480
C	0.097804	4.984761	0.810308	C	-1.254686	1.137323	2.565676
C	0.467462	6.308451	1.192376	H	-0.289825	0.690460	2.333018
C	-0.333385	7.040055	2.082893	H	-1.158424	2.021557	3.194695
C	1.639789	6.877842	0.670014	H	-1.947022	0.416915	3.000712
C	0.040197	8.328247	2.444522				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298294 hartree
Thermal correction to Gibbs free energy = 0.241994 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10155.6681155 hartree

Entrance2 of the reaction for 7k:

Atom	x	y	z	Atom	x	y	z
C	-2.390758	-4.225539	-1.625987	H	-1.092831	6.491192	2.638693
C	-2.741912	-3.140983	-0.855687	C	1.931271	8.223005	0.932835
C	-1.994711	-1.942640	-0.911244	H	2.126785	6.404928	-0.211272
C	-0.861542	-1.848611	-1.772780	C	1.207933	8.890638	1.921207
C	-0.516373	-2.977323	-2.562017	H	-0.440185	8.790122	3.305002
C	-1.259790	-4.124373	-2.486300	H	2.777505	8.706661	0.456614
C	-0.123493	-0.643880	-1.809086	H	1.492890	9.895888	2.213939
C	-0.519356	0.403259	-1.009121	N	-2.390217	-0.890036	-0.127488
C	-1.669113	0.173122	-0.207144	Se	-2.077170	1.748147	0.833992
C	-0.516927	2.559215	0.042660	I	1.750332	2.291315	-1.905550
C	0.072336	1.720901	-0.843840	H	-0.987858	-4.984165	-3.092052
H	-3.596310	-3.176067	-0.187109	C	-3.169471	-5.511040	-1.580871
H	0.344277	-2.914198	-3.220776	H	-3.564513	-5.756842	-2.571823
H	0.744433	-0.554296	-2.457075	H	-2.524483	-6.340409	-1.273465
C	-0.173191	3.861438	0.425400	H	-4.005175	-5.445781	-0.881522
C	0.110356	4.986643	0.782127	C	-1.301338	1.163813	2.550152
C	0.476745	6.309399	1.171653	H	-0.336351	0.706079	2.345001
C	-0.249593	6.983032	2.165728	H	-1.211821	2.053233	3.170326
C	1.571698	6.935677	0.555146	H	-2.008432	0.456342	2.978830
C	0.120277	8.270088	2.535444	I	-0.244734	0.154931	5.655991

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298393 hartree
Thermal correction to Gibbs free energy = 0.235746 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3337723 hartree

TS2 of the reaction for 7k:

Atom	x	y	z	Atom	x	y	z
C	-2.416733	-4.197651	-1.619762	H	-1.250254	6.626630	2.466695
C	-2.780519	-3.109961	-0.862213	C	1.980328	8.189270	0.994089
C	-2.025227	-1.912789	-0.897174	H	2.213572	6.322595	-0.061501
C	-0.868786	-1.830892	-1.728887	C	1.193899	8.918937	1.885513
C	-0.509095	-2.965734	-2.505555	H	-0.578954	8.926762	3.109369
C	-1.260610	-4.107364	-2.449206	H	2.884475	8.625340	0.582589
C	-0.123501	-0.632710	-1.747139	H	1.487217	9.924814	2.167773
C	-0.537231	0.421442	-0.963501	N	-2.435527	-0.861851	-0.124762
C	-1.712973	0.209955	-0.187231	Se	-2.127916	1.766372	0.843275
C	-0.572400	2.572909	0.074499	I	1.763432	2.297756	-1.807788
C	0.052921	1.733612	-0.790180	H	-0.978100	-4.970714	-3.045129
H	-3.653775	-3.138427	-0.217798	C	-3.206206	-5.477611	-1.595071
H	0.370319	-2.908911	-3.140029	H	-3.577448	-5.721204	-2.595851
H	0.764458	-0.550863	-2.368734	H	-2.576692	-6.312505	-1.270639
C	-0.225424	3.881204	0.446320	H	-4.059810	-5.405725	-0.918118
C	0.064302	5.009167	0.787549	C	-1.132971	0.971647	2.746524
C	0.440726	6.334431	1.162352	H	-0.184841	0.727500	2.287572
C	-0.348610	7.070972	2.058755	H	-1.210998	1.877569	3.330182
C	1.609780	6.900861	0.630128	H	-1.846774	0.178480	2.922936
C	0.031849	8.358818	2.415623	I	0.103282	-0.039250	5.073053

Number of imaginary frequencies = 1 (-445.7607 cm^{-1})
Zero-point vibrational correction = 0.297455 hartree
Thermal correction to Gibbs free energy = 0.235711 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3270958 hartree

Product of the reaction for 7k:

Atom	x	y	z	Atom	x	y	z
C	-2.330568	-4.226658	-1.679547	C	1.583327	6.906295	0.515517
C	-2.657746	-3.173746	-0.862308	C	0.180329	8.267026	2.509582
C	-1.919606	-1.960561	-0.892517	H	-1.017168	6.482367	2.676673
C	-0.816560	-1.837302	-1.789920	C	1.944977	8.203010	0.859679
C	-0.493504	-2.940264	-2.630298	H	2.120075	6.365940	-0.257482
C	-1.226428	-4.092297	-2.574585	C	1.245800	8.884888	1.855525
C	-0.091538	-0.630414	-1.808139	H	-0.363848	8.797039	3.284352
C	-0.469527	0.390889	-0.961924	H	2.773967	8.683169	0.350265
C	-1.594133	0.145598	-0.110739	H	1.531177	9.897488	2.121619

C	-0.498409	2.499045	0.131743	N	-2.295132	-0.953107	-0.057359
C	0.103281	1.702905	-0.792728	Se	-1.971405	1.648467	0.975310
H	-3.490878	-3.237944	-0.168609	I	1.746289	2.331297	-1.892413
H	0.345218	-2.847016	-3.314362	H	-0.972661	-4.929097	-3.219659
H	0.753658	-0.510845	-2.481660	C	-3.104846	-5.516777	-1.656786
C	-0.146859	3.813866	0.493168	H	-3.537401	-5.726362	-2.640697
C	0.141847	4.946942	0.816422	H	-2.449696	-6.357560	-1.405979
C	0.511422	6.280906	1.171588	H	-3.914984	-5.481539	-0.925284
C	-0.189625	6.970462	2.172754				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.259827 hartree
Thermal correction to Gibbs free energy = 0.207324 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10115.9872590 hartree

Reaction for 7l

Reactant1 of the reaction for 7l:

Atom	x	y	z	Atom	x	y	z
C	-1.760728	-4.136464	-2.044334	C	0.487950	7.452874	1.952109
C	-2.245622	-3.459842	-0.948165	C	1.904030	7.344313	-0.016737
C	-1.773698	-2.133622	-0.713478	C	0.895799	8.763921	2.165883
C	-0.831629	-1.545840	-1.599591	H	-0.217916	6.975851	2.623975
C	-0.359351	-2.281759	-2.716841	C	2.305177	8.655815	0.206194
C	-0.819777	-3.554483	-2.929668	H	2.289323	6.783383	-0.861780
C	-0.410458	-0.226290	-1.326000	C	1.803259	9.367012	1.295545
C	-0.910187	0.446719	-0.230084	H	0.504518	9.316850	3.013643
C	-1.836924	-0.251955	0.616775	H	3.011110	9.124459	-0.471749
C	-0.170827	2.941808	0.217398	H	2.119083	10.391220	1.466138
C	-0.526360	1.794618	0.032072	N	-2.244811	-1.468091	0.381867
H	-2.109086	-5.147379	-2.237394	Se	-2.578456	0.633189	2.148221
C	-3.242317	-4.073204	-0.005361	C	-0.941167	0.747209	3.205509
H	0.360019	-1.821641	-3.387829	H	-1.220659	1.238204	4.138000
H	-0.466726	-4.127857	-3.780702	H	-0.193129	1.343559	2.684479
H	0.296938	0.263280	-1.989490	H	-0.578305	-0.258298	3.410417
C	0.224859	4.236983	0.437331	H	-3.499071	-5.086130	-0.322743
C	0.575832	5.384053	0.631250	H	-4.157399	-3.475366	0.038835
C	0.990897	6.733312	0.856945	H	-2.842778	-4.113064	1.012132

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.297233 hartree
Thermal correction to Gibbs free energy = 0.243686 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -3265.33217354 hartree

Entrance1 of the reaction for 7l:

Atom	x	y	z	Atom	x	y	z
C	-0.041955	0.057801	-0.035524	H	3.317746	0.118333	-0.641260
C	-0.072078	0.000867	1.339485	H	4.546590	0.106081	1.550083
C	1.171735	-0.017361	2.039358	H	4.330518	-1.031652	6.779703
C	2.393669	0.027234	1.316291	H	3.570024	-2.161695	5.620461
C	2.376294	0.083943	-0.101285	H	2.966517	-2.071475	7.292049
C	1.175298	0.098433	-0.760317	C	8.007413	0.382800	6.148075
C	3.591074	0.036947	2.062213	C	9.227452	0.486221	6.883943
N	1.143750	-0.097003	3.400493	C	10.459671	0.405353	6.216229
C	3.551755	-0.008241	3.441412	C	9.198090	0.668663	8.275433
C	2.263470	-0.105422	4.071529	C	11.644043	0.505894	6.935763
C	4.756744	0.094908	4.193541	C	11.611105	0.687352	8.318154
C	5.801716	0.195246	4.811125	C	10.388762	0.768630	8.984782
C	6.971989	0.295973	5.518192	H	10.475047	0.264695	5.140678
I	4.467758	3.162401	5.242670	H	8.242444	0.731119	8.785042
I	3.956132	5.783307	5.672716	H	12.594945	0.442802	6.417135
Se	2.065135	-0.154702	5.976803	H	12.538461	0.765911	8.876177
C	3.399114	-1.500981	6.470353	H	10.363147	0.910326	10.060126
H	-0.980190	0.071850	-0.583103	H	-2.216263	-0.020932	1.432876
C	-1.360546	-0.045108	2.111091	H	-1.432935	0.801400	2.800257
H	1.146856	0.142458	-1.844037	H	-1.418149	-0.952463	2.719396

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298026 hartree
Thermal correction to Gibbs free energy = 0.232051 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3134980 hartree

TS1 of the reaction for 7l:

Atom	x	y	z	Atom	x	y	z
C	0.045681	-0.044292	-0.035070	H	3.418265	-0.048810	-0.569723
C	-0.014725	-0.017071	1.340157	H	4.601863	-0.053457	1.631091
C	1.213754	0.002097	2.063324	H	1.186829	-2.211799	6.003585
C	2.453590	-0.012228	1.368890	H	-0.010470	-0.979277	5.473707
C	2.465644	-0.038596	-0.048979	H	0.384805	-1.161635	7.215282
C	1.278365	-0.053635	-0.733302	C	5.862005	-0.473958	7.994650
C	3.640590	-0.018202	2.135240	C	6.428346	-0.598662	9.288606
N	1.160959	0.049871	3.426489	C	6.666787	-1.874490	9.830724
C	3.576630	-0.007135	3.509063	C	6.749091	0.555138	10.026433
C	2.269586	0.047664	4.102985	C	7.220204	-1.987934	11.098142
C	4.724296	-0.099199	4.385739	C	7.536219	-0.840649	11.827481
C	4.827677	-0.238588	5.650420	C	7.301146	0.427128	11.293024
C	5.385744	-0.363531	6.874417	H	6.416084	-2.755895	9.250637
I	6.850649	-0.047646	3.479241	H	6.561588	1.532728	9.595802
I	9.437230	0.049732	1.968801	H	7.406646	-2.969694	11.519522
Se	2.155510	0.131722	6.017258	H	7.969024	-0.935050	12.818062

C	0.766332	-1.226791	6.197418	H	7.550217	1.314117	11.865147
H	-0.880153	-0.058683	-0.603180	H	-2.160155	-0.018612	1.388972
C	-1.319371	-0.006782	2.085780	H	-1.399760	0.881451	2.719332
H	1.273661	-0.073992	-1.817994	H	-1.399014	-0.875970	2.745976

Number of imaginary frequencies = 1 (-158.9396 cm^{-1})
Zero-point vibrational correction = 0.296567 hartree
Thermal correction to Gibbs free energy = 0.234663 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.2983839 hartree

IM of the reaction for 7l:

Atom	x	y	z	Atom	x	y	z
C	-2.419456	-4.181618	-1.660645	C	1.619047	6.866166	0.633114
C	-2.823896	-3.129239	-0.870117	C	0.116180	8.322365	2.485438
C	-2.058121	-1.929960	-0.916332	H	-1.182889	6.603984	2.561156
C	-0.908796	-1.832917	-1.757828	C	2.014694	8.146902	0.997789
C	-0.537201	-2.946576	-2.553237	H	2.192610	6.289394	-0.085098
C	-1.282630	-4.095538	-2.500277	C	1.266173	8.875351	1.922294
C	-0.168544	-0.625825	-1.772700	H	-0.465321	8.890041	3.204178
C	-0.573064	0.420612	-0.977575	H	2.908802	8.577646	0.559788
C	-1.737452	0.184856	-0.199605	H	1.579339	9.875358	2.204063
C	-0.576747	2.566859	0.073485	N	-2.460618	-0.876798	-0.136746
C	0.030829	1.734069	-0.805099	Se	-2.161654	1.762705	0.837890
H	-2.989786	-5.105619	-1.640371	I	1.755911	2.303766	-1.842034
C	-4.030375	-3.212604	0.021656	C	-1.419548	1.172397	2.545201
H	0.336063	-2.870037	-3.193102	H	-0.446108	0.725767	2.351138
H	-1.004981	-4.952221	-3.105038	H	-1.344955	2.057038	3.176436
H	0.711075	-0.533675	-2.404425	H	-2.127039	0.453191	2.956693
C	-0.236572	3.867980	0.468840	I	4.605129	3.223950	-3.540794
C	0.062647	4.990220	0.821521	H	-4.499995	-4.194608	-0.061042
C	0.461869	6.307543	1.199215	H	-4.766228	-2.448336	-0.245190
C	-0.289816	7.042447	2.128628	H	-3.756392	-3.042156	1.066977

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298824 hartree
Thermal correction to Gibbs free energy = 0.237017 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3350576 hartree

Reactant2 of the reaction for 7l:

Atom	x	y	z	Atom	x	y	z
C	-2.406649	-4.207432	-1.648074	C	1.578141	6.896646	0.604480
C	-2.803888	-3.152105	-0.857424	C	0.070676	8.283087	2.506417
C	-2.036372	-1.954873	-0.914043	H	-1.172676	6.524189	2.588881
C	-0.893181	-1.862009	-1.765467	C	1.941619	8.184607	0.975939
C	-0.529496	-2.978327	-2.560350	H	2.153563	6.346498	-0.132683

C	-1.276571	-4.125787	-2.497027	H	1.190371	8.877994	1.925024
C	-0.151584	-0.656374	-1.790057	H	-0.511968	8.824134	3.244285
C	-0.549106	0.391308	-0.993442	H	2.811912	8.649152	0.524868
C	-1.706887	0.161456	-0.205166	H	1.477894	9.884119	2.211983
C	-0.547025	2.547405	0.061745	N	-2.430305	-0.898404	-0.135029
C	0.046851	1.707179	-0.820068	Se	-2.123846	1.741672	0.831952
H	-2.977779	-5.130615	-1.620482	I	1.736222	2.272159	-1.863842
C	-4.003365	-3.230644	0.043878	C	-1.371342	1.159613	2.537730
H	0.338460	-2.906061	-3.207801	H	-0.406335	0.697131	2.339308
H	-1.005360	-4.984992	-3.101005	H	-1.281454	2.049823	3.159100
H	0.721863	-0.568968	-2.430913	H	-2.086382	0.454038	2.959887
C	-0.205330	3.848002	0.449332	H	-3.720970	-3.056092	1.086193
C	0.080458	4.973648	0.803599	H	-4.474146	-4.212557	-0.031085
C	0.451022	6.296254	1.188250	H	-4.740559	-2.467092	-0.221060
C	-0.303440	6.995626	2.142919				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298747 hartree
Thermal correction to Gibbs free energy = 0.243454 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10155.6679030 hartree

Entrance2 of the reaction for 7l:

Atom	x	y	z	Atom	x	y	z
C	-2.431752	-4.174929	-1.666244	C	1.602053	6.920856	0.572854
C	-2.833734	-3.106816	-0.895945	C	0.126711	8.274507	2.522346
C	-2.052083	-1.917867	-0.948314	H	-1.111168	6.511417	2.600191
C	-0.889183	-1.848076	-1.774078	C	1.970236	8.203520	0.958000
C	-0.521018	-2.977193	-2.549162	H	2.166179	6.382709	-0.181709
C	-1.282369	-4.115191	-2.491151	C	1.234989	8.880693	1.930990
C	-0.132645	-0.651989	-1.793156	H	-0.442877	8.801917	3.280084
C	-0.535850	0.408034	-1.016242	H	2.832491	8.676076	0.499706
C	-1.714767	0.202533	-0.251299	H	1.526778	9.882226	2.229668
C	-0.532574	2.571094	0.019709	N	-2.451825	-0.849878	-0.189393
C	0.072694	1.717205	-0.840549	Se	-2.133296	1.792443	0.763031
H	-3.013187	-5.091758	-1.640178	I	1.796867	2.249115	-1.845867
C	-4.051059	-3.162996	-0.017168	C	-1.424343	1.212506	2.509633
H	0.362917	-2.921640	-3.176483	H	-0.457907	0.743104	2.342046
H	-1.007220	-4.984143	-3.079329	H	-1.346900	2.105840	3.125615
H	0.757410	-0.582252	-2.412975	H	-2.153441	0.515744	2.918545
C	-0.179410	3.869266	0.407646	I	-0.420044	0.213775	5.633762
C	0.111065	4.991105	0.769415	H	-4.530724	-4.140892	-0.090272
C	0.486306	6.309117	1.166286	H	-4.775015	-2.394456	-0.303610
C	-0.251996	6.992288	2.144929	H	-3.786028	-2.979428	1.028132

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.298858 hartree

Thermal correction to Gibbs free energy = 0.236914 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3337931 hartree

TS2 of the reaction for 7l:

Atom	x	y	z	Atom	x	y	z
C	-2.477753	-4.129317	-1.686695	C	1.656108	6.877470	0.666366
C	-2.892702	-3.056873	-0.931719	C	0.047124	8.373935	2.391411
C	-2.097841	-1.872753	-0.954901	H	-1.270820	6.668114	2.403615
C	-0.907768	-1.818602	-1.742444	C	2.039763	8.159639	1.038627
C	-0.525572	-2.954440	-2.504144	H	2.271648	6.284340	-0.001941
C	-1.299012	-4.083770	-2.472667	C	1.237876	8.908433	1.899947
C	-0.139741	-0.632548	-1.736022	H	-0.575678	8.956925	3.061612
C	-0.559919	0.434813	-0.975892	H	2.966155	8.575901	0.657201
C	-1.768228	0.251335	-0.244860	H	1.541594	9.909288	2.188962
C	-0.590826	2.591764	0.049581	N	-2.511464	-0.806435	-0.206989
C	0.050652	1.735772	-0.786332	Se	-2.190147	1.820552	0.763694
H	-3.070618	-5.039354	-1.680399	I	1.813727	2.255786	-1.734914
C	-4.140335	-3.099514	-0.095509	C	-1.276573	1.011880	2.700321
H	0.379985	-2.907704	-3.101018	H	-0.316526	0.753451	2.275345
H	-1.013523	-4.956308	-3.050695	H	-1.360918	1.917821	3.283176
H	0.772942	-0.573118	-2.323466	H	-2.007276	0.228922	2.851820
C	-0.231579	3.894514	0.429118	I	-0.130133	-0.024157	5.063518
C	0.068487	5.017883	0.776516	H	-4.630704	-4.070653	-0.188138
C	0.458153	6.336844	1.159728	H	-4.843520	-2.319884	-0.403141
C	-0.346775	7.092615	2.025780	H	-3.909283	-2.921928	0.959000

Number of imaginary frequencies = 1 (-446.7170 cm^{-1})
Zero-point vibrational correction = 0.297741 hartree
Thermal correction to Gibbs free energy = 0.236600 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17046.3270995 hartree

Product of the reaction for 7l:

Atom	x	y	z	Atom	x	y	z
C	-2.356609	-4.180084	-1.733738	C	0.517388	6.274051	1.183069
C	-2.730027	-3.152270	-0.902483	C	-0.198618	6.976217	2.164665
C	-1.962815	-1.944951	-0.926669	C	1.613734	6.882503	0.551871
C	-0.839598	-1.832992	-1.802099	C	0.180828	8.268613	2.506891
C	-0.496660	-2.928318	-2.642894	H	-1.045018	6.501102	2.649328
C	-1.241319	-4.074587	-2.606126	C	1.984690	8.175169	0.901233
C	-0.103176	-0.631153	-1.803122	H	2.161874	6.332301	-0.206045
C	-0.485028	0.394647	-0.965572	C	1.270598	8.869668	1.877595
C	-1.627556	0.160496	-0.136447	H	-0.374873	8.808509	3.266504
C	-0.513675	2.502228	0.127828	H	2.832636	8.642250	0.411216
C	0.097595	1.701087	-0.786029	H	1.563323	9.879053	2.147883
H	-2.931458	-5.101986	-1.724365	N	-2.339010	-0.931338	-0.100167

C	-3.910023	-3.259357	0.021815	Se	-2.009821	1.666146	0.944546
H	0.358858	-2.833162	-3.305085	I	1.763326	2.315282	-1.858843
H	-0.985611	-4.913905	-3.244493	H	-4.388213	-4.236333	-0.076585
C	0.756178	-0.521080	-2.460174	H	-4.648853	-2.482375	-0.196472
C	-0.156102	3.813761	0.495344	H	-3.604498	-3.120263	1.063160
C	0.138917	4.944001	0.822705				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.260116 hartree
Thermal correction to Gibbs free energy = 0.208042 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10115.9873339 hartree

Reaction for 7m

Reactant1 of the reaction for 7m:

Atom	x	y	z	Atom	x	y	z
C	-1.755433	-4.140739	-2.046979	C	0.988884	6.740958	0.856439
C	-2.219833	-3.442541	-0.959932	C	0.492943	7.455583	1.958009
C	-1.763432	-2.123849	-0.716173	C	1.894505	7.356658	-0.021764
C	-0.825739	-1.536335	-1.606528	C	0.900350	8.766447	2.173682
C	-0.361634	-2.280022	-2.722100	H	-0.207128	6.974922	2.633335
C	-0.818505	-3.555870	-2.935633	C	2.295249	8.667935	0.203121
C	-0.405189	-0.215457	-1.335169	H	2.274368	6.799495	-0.871744
C	-0.904509	0.453354	-0.237152	C	1.800379	9.374210	1.298889
C	-1.829537	-0.247033	0.613848	H	0.514590	9.315563	3.026436
C	-0.168883	2.949090	0.212421	H	2.995402	9.140233	-0.478269
C	-0.522453	1.801432	0.026378	H	2.115929	10.398237	1.471037
H	-2.105691	-5.151068	-2.232033	N	-2.237272	-1.463599	0.383103
H	-2.935718	-3.870545	-0.266046	Se	-2.566687	0.640782	2.146036
H	0.354709	-1.821863	-3.397976	C	-0.926574	0.749046	3.199365
H	-0.464077	-4.124921	-3.788750	H	-1.202811	1.239137	4.133331
H	0.299269	0.276703	-1.999768	H	-0.178354	1.344500	2.677490
C	0.224952	4.244555	0.433625	H	-0.565940	-0.257788	3.401682
C	0.574679	5.391761	0.628993				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.269174 hartree
Thermal correction to Gibbs free energy = 0.217482 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -3226.02391851 hartree

Entrance1 of the reaction for 7m:

Atom	x	y	z	Atom	x	y	z
C	-0.046679	0.024240	-0.053925	H	-0.968034	-0.060357	1.890583

C	-0.047219	-0.026317	1.318166	H	1.149040	0.103488	-1.861472
C	1.179121	-0.039144	2.027850	H	3.312484	0.088174	-0.657373
C	2.400011	0.003894	1.303464	H	4.554754	0.086063	1.538912
C	2.372622	0.054509	-0.114178	H	4.331826	-1.035919	6.771237
C	1.171942	0.064164	-0.777638	H	3.570290	-2.167534	5.614000
C	3.598239	0.017927	2.049251	C	2.965518	-2.072319	7.284827
N	1.143838	-0.112653	3.390499	C	8.004764	0.381783	6.141471
C	3.554524	-0.021868	3.427953	C	9.223270	0.488525	6.879348
C	2.264403	-0.117136	4.059399	C	10.456769	0.407257	6.214088
C	4.757917	0.084568	4.182144	C	9.191101	0.674387	8.270333
C	5.801846	0.187720	4.800955	C	11.639669	0.510669	6.935631
C	6.970700	0.291863	5.509777	C	11.603958	0.695371	8.317539
I	4.468932	3.158313	5.218679	H	10.380336	0.777222	8.981679
I	3.958527	5.781380	5.636675	H	10.474261	0.264060	5.138887
Se	2.068658	-0.156827	5.964968	H	8.234462	0.737176	8.777989
C	3.399906	-1.504501	6.462224	H	12.591582	0.447253	6.418945
H	-0.987129	0.033240	-0.595181	H	12.530176	0.776096	8.877152
H	-0.046679	0.024240	-0.053925				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.269994 hartree
Thermal correction to Gibbs free energy = 0.205815 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17007.0051576 hartree

TS1 of the reaction for 7m:

Atom	x	y	z	Atom	x	y	z
C	0.054848	-0.035295	-0.056804	H	1.293975	-0.073457	-1.835228
C	0.020473	-0.007058	1.315833	H	3.428075	-0.058284	-0.580166
C	1.229522	0.004005	2.051795	H	4.619017	-0.062877	1.627247
C	2.469793	-0.015951	1.359020	H	1.208555	-2.221997	5.991813
C	2.475549	-0.043148	-0.058942	H	-0.001268	-0.999020	5.468705
C	1.290527	-0.052553	-0.750726	H	0.402420	-1.180398	7.207934
C	3.655935	-0.024878	2.127626	C	5.862248	-0.473408	7.991862
N	1.166768	0.050343	3.416005	C	6.425012	-0.596485	9.287545
C	3.585266	-0.012137	3.500596	C	6.663656	-1.871631	9.831145
C	2.275046	0.045043	4.092897	C	6.741767	0.558251	10.025613
C	4.730538	-0.103638	4.380401	C	7.213317	-1.983479	11.100339
C	4.833645	-0.240682	5.644877	C	7.525352	-0.835284	11.829953
C	5.388787	-0.364295	6.870354	C	7.290073	0.431818	11.293992
I	6.861643	-0.054087	3.477774	H	6.416015	-2.753757	9.250840
I	9.448200	0.042252	1.973164	H	6.554106	1.535300	9.593828
Se	2.158322	0.128879	6.007143	H	7.399880	-2.964705	11.522902
C	0.780554	-1.240824	6.188497	H	7.955164	-0.928433	12.821954
H	-0.871996	-0.043258	-0.620882	H	7.536023	1.319517	11.866359
H	-0.914002	0.009939	1.866319				

Number of imaginary frequencies = 1 (-158.4324 cm^{-1})
Zero-point vibrational correction = 0.268532 hartree
Thermal correction to Gibbs free energy = 0.208468 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17006.9900914 hartree

IM of the reaction for 7m:

Atom	x	y	z	Atom	x	y	z
C	-2.409581	-4.195139	-1.694898	C	-0.299332	7.029767	2.128478
C	-2.795052	-3.130672	-0.917714	C	1.613174	6.859010	0.636878
C	-2.044941	-1.932872	-0.945718	C	0.104507	8.309282	2.489157
C	-0.891358	-1.836089	-1.780150	H	-1.192887	6.589327	2.557984
C	-0.522470	-2.954085	-2.571486	C	2.006611	8.139314	1.005400
C	-1.266535	-4.106220	-2.527250	H	2.188980	6.284476	-0.081333
C	-0.150532	-0.628682	-1.789328	C	1.255180	8.864791	1.929886
C	-0.562884	0.414065	-0.994032	H	-0.479208	8.874666	3.207903
C	-1.733287	0.176754	-0.222241	H	2.901242	8.572035	0.570433
C	-0.575115	2.558752	0.061113	H	1.566615	9.864478	2.214686
C	0.038410	1.727909	-0.815121	N	-2.457939	-0.884028	-0.163733
H	-2.983798	-5.115207	-1.675026	Se	-2.164587	1.752786	0.814236
H	-3.667031	-3.174597	-0.274459	I	1.769429	2.301350	-1.840428
H	0.354338	-2.879691	-3.207114	C	-1.434062	1.161052	2.526043
H	-0.980906	-4.959096	-3.133355	H	-0.458526	0.716158	2.338788
H	0.733000	-0.533651	-2.415066	H	-1.365564	2.045338	3.158465
C	-0.238129	3.859288	0.460889	H	-2.143572	0.440600	2.931762
C	0.058536	4.981063	0.817213	I	4.625615	3.227939	-3.520636
C	0.455290	6.297886	1.199062				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.270828 hartree
Thermal correction to Gibbs free energy = 0.210998 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17007.0263633 hartree

Reactant2 of the reaction for 7m:

Atom	x	y	z	Atom	x	y	z
C	-2.432574	-4.192432	-1.679895	C	0.475262	6.294099	1.200390
C	-2.806705	-3.120913	-0.906667	C	-0.335937	7.032610	2.075751
C	-2.044275	-1.931636	-0.941203	C	1.663758	6.851893	0.702578
C	-0.890266	-1.850096	-1.777602	H	0.043708	8.316244	2.447040
C	-0.533701	-2.974791	-2.564799	C	-1.253315	6.594511	2.454098
C	-1.289906	-4.118771	-2.514210	H	2.032178	8.136395	1.081034
C	-0.137232	-0.650802	-1.792604	C	2.282285	6.271886	0.025710
C	-0.539168	0.397902	-1.000181	H	1.224939	8.868488	1.951820
C	-1.710821	0.177806	-0.226331	H	-0.582884	8.887711	3.123367
C	-0.535767	2.554593	0.054878	H	2.950017	8.568066	0.696519
C	0.064109	1.709421	-0.818042	N	1.516755	9.871665	2.244728

H	-3.015873	-5.106547	-1.655435	Se	-2.445350	-0.874814	-0.164258
H	-3.678195	-3.153267	-0.262252	I	-2.130301	1.762146	0.802533
H	0.342776	-2.912864	-3.202140	C	1.772939	2.261337	-1.836649
H	-1.014241	-4.977212	-3.116937	H	-1.408439	1.179015	2.521181
H	0.745511	-0.569382	-2.421302	H	-0.442925	0.710720	2.340076
C	-0.189140	3.851956	0.448781	H	-1.323793	2.070719	3.141090
C	0.099921	4.975010	0.808636	C	-2.134159	0.478890	2.933941
C	-2.432574	-4.192432	-1.679895				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.270804 hartree
Thermal correction to Gibbs free energy = 0.217737 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10116.3590938 hartree

Entrance2 of the reaction for 7m:

Atom	x	y	z	Atom	x	y	z
C	-2.429880	-4.182540	-1.708301	C	-0.266175	6.983517	2.138707
C	-2.812700	-3.101809	-0.952821	C	1.603260	6.912148	0.584838
C	-2.042887	-1.916502	-0.982320	C	0.109398	8.265339	2.520549
C	-0.872177	-1.850024	-1.795949	H	-1.129985	6.502745	2.585213
C	-0.506668	-2.984244	-2.565633	C	1.968219	8.194405	0.974341
C	-1.270148	-4.123296	-2.520260	H	2.174505	6.374175	-0.164470
C	-0.112155	-0.655447	-1.806400	C	1.223726	8.871329	1.940443
C	-0.523698	0.402028	-1.031053	H	-0.467359	8.792577	3.272957
C	-1.711380	0.197519	-0.276077	H	2.835158	8.666843	0.524855
C	-0.528515	2.564284	0.007521	H	1.513011	9.872557	2.242566
C	0.083915	1.710726	-0.847921	N	-2.452949	-0.852068	-0.221785
H	-3.018389	-5.093424	-1.686077	Se	-2.135822	1.786044	0.737182
H	-3.695757	-3.123544	-0.323836	I	1.817842	2.242503	-1.836288
H	0.383630	-2.933111	-3.184661	C	-1.439147	1.204010	2.488506
H	-0.986803	-4.989211	-3.108691	H	-0.471450	0.735002	2.327366
H	0.784122	-0.584962	-2.417022	H	-1.366001	2.097312	3.105075
C	-0.178023	3.861782	0.399831	H	-2.171183	0.507186	2.892007
C	0.109450	4.983167	0.765433	I	-0.437717	0.214557	5.614628
C	0.481424	6.300639	1.166943				

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.270833 hartree
Thermal correction to Gibbs free energy = 0.210618 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17007.0249159 hartree

TS2 of the reaction for 7m:

Atom	x	y	z	Atom	x	y	z
C	-2.469378	-4.142892	-1.717659	C	-0.359995	7.082589	2.022015
C	-2.863122	-3.059469	-0.973711	C	1.651558	6.869453	0.674977

C	-2.083809	-1.877113	-0.978318	C	0.030477	8.364217	2.390214
C	-0.890251	-1.823184	-1.759509	H	-1.286005	6.657190	2.393982
C	-0.512428	-2.962537	-2.518599	C	2.031721	8.151909	1.049773
C	-1.285155	-4.094644	-2.496647	H	2.271737	6.276938	0.010419
C	-0.121419	-0.637013	-1.747201	C	1.223776	8.899834	1.906185
C	-0.548511	0.426485	-0.986283	H	-0.596998	8.946594	3.056574
C	-1.761844	0.241271	-0.260289	H	2.960085	8.569082	0.674186
C	-0.587315	2.582415	0.042090	H	1.524754	9.900938	2.197197
C	0.059282	1.728137	-0.791473	N	-2.506711	-0.815278	-0.227113
H	-3.066817	-5.048406	-1.712835	Se	-2.189071	1.808696	0.748412
H	-3.764309	-3.073992	-0.370461	I	1.826576	2.251842	-1.730127
H	0.396056	-2.918024	-3.111568	C	-1.280045	1.004936	2.687712
H	-0.992591	-4.963133	-3.076884	H	-0.321578	0.738011	2.264444
H	0.794309	-0.574620	-2.329489	H	-1.358168	1.914772	3.265397
C	-0.231694	3.885119	0.424811	H	-2.014639	0.227060	2.846297
C	0.064988	5.008587	0.774842	I	-0.133805	-0.021283	5.057171
C	0.451032	6.327729	1.160866				

Number of imaginary frequencies = 1 (-446.4279 cm^{-1})
Zero-point vibrational correction = 0.269702 hartree
Thermal correction to Gibbs free energy = 0.210438 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -17007.0183867 hartree

Product of the reaction for 7m:

Atom	x	y	z	Atom	x	y	z
C	-2.340761	-4.197846	-1.751792	C	-0.155150	3.805121	0.489234
C	-2.691432	-3.159284	-0.929657	C	0.136555	4.935340	0.819625
C	-1.943895	-1.951688	-0.942243	C	0.511524	6.265515	1.182953
C	-0.824403	-1.835815	-1.821378	C	-0.205939	6.963401	2.166552
C	-0.488460	-2.933528	-2.661896	C	1.605973	6.878297	0.552667
C	-1.228082	-4.085302	-2.627677	C	0.170302	8.255955	2.511692
C	-0.090915	-0.631447	-1.822519	H	-1.050890	6.484905	2.650407
C	-0.476212	0.388712	-0.980380	C	1.973736	8.171062	0.905002
C	-1.617173	0.149138	-0.147338	H	2.155195	6.331311	-0.206788
C	-0.509343	2.493585	0.118877	C	1.258251	8.861314	1.883348
C	0.102332	1.696869	-0.798341	H	-0.386463	8.792607	3.272816
H	-2.915776	-5.118023	-1.737620	H	2.820245	8.641552	0.415771
H	-3.537369	-3.224088	-0.253481	H	1.548461	9.870810	2.155921
H	0.364116	-2.837470	-3.328067	N	-2.326174	-0.943883	-0.109714
H	-0.967819	-4.919476	-3.270614	Se	-2.001077	1.651228	0.937405
H	0.766321	-0.515533	-2.481233	I	1.763821	2.319445	-1.872843

Number of imaginary frequencies = 0
Zero-point vibrational correction = 0.232049 hartree
Thermal correction to Gibbs free energy = 0.181752 hartree
M06-2X/6-311+G**+Midi!//M06-2X/6-31G*+Midi! electronic energy = -10076.6789749 hartree