Supporting Information

Fine Tuning of the Orifice Size of an Open-Cage Fullerene by Placing Selenium in the Rim: Insertion/Release of Molecular Hydrogen

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Content

[1] Gaussian 03, Revision B.05, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Pittsburgh PA, 2003.

Experimental Section

General method.

All reactions were performed under argon. Dry ODCB was distilled from CaH_2 under argon. 90% sodium *t*-butylthiolate (Aldrich), 90% sodium isopropylthiolate (Fluka), 95% sodium methylthiolate (Aldrich), anhydrous benzonitrile (Aldrich) and selenium powder (100 mesh, Aldrich) were used as received.

Synthesis of compound 2. To a stirred solution of **1** (207 mg, 0.200 mmol) and S_8 (256 mg, 1 mmol) in 50 mL dry benzonitrile at ambient temperature was added 2.2 equivalents of 90% sodium *t*-butylthiolate (50.1 mg, 0.447 mmol). The color of the resulting mixture turned from brown to black immediately. After 3 h, when the reaction was completed, the reaction mixture was worked up by addition of I_2 and then washed with sat. sodium thiosulfate solution. After the organic layer was separated from aqueous layer and dried with Na_2SO_4, the organic solution was evaporated under reduced pressure. The residue was chromatographed over silica gel to afford 171 mg of **2**. Yield: 80%. The spectral data of **2** were identical to those of the product obtained by the use of TDAE. The ^{1}H NMR spectrum of H_2@**2** was also identical to that which had been prepared using TDAE followed by hydrogen insertion.

Synthesis of compound 3. A solution of **1** (328 mg, 0.317 mmol) and selenium powder (260 mg, 3.29 mmol) in 150 mL of ODCB freshly distilled under argon was heated at 180 ^{o}C for 2 h. To the solution, 95% sodium methylthiolate (49.8 mg, 0.675 mmol) was added by a weighing boat and the mixture was heated at 180 ^{o}C for 4 h. The reaction course was monitored by HPLC equipped with an analytical Buckyprep column. The reaction mixture was cooled and directly poured to a short silica gel plug (5 cm x 5 cm) to remove baseline materials. The eluted reaction mixture was subjected to separation by Buckyprep

column (50 ^{o}C, flow rate = 8 ml/min toluene, Φ = 20 mm) to give 163 mg of open-cage fullerene **3** as an orange-brown solid. Yield: 46% (53% based on recovered 43 mg of **1**). From the second fraction was obtained 33.1 mg of **2** (yield: 9.8%). Spectral data of **3**: ^{77}Se NMR (ODCB-d_4, 75.5 MHz): δ 195.7 (referring to dibenzyl diselenide as external standard; dibenzyl diselenide has chemical shift at δ 411 with respect to dimethyl selenide at 0 ppm); ^{1}H NMR (ODCB-d_4, 400 MHz) δ 6.78 (t, J = 7.5 Hz, 1H), 7.02 (dd, J = 4.4, 7.1 Hz, 1H), 7.24 (t, J = 7.1 Hz, 1H), 7.31 (t, J = 7.3 Hz, 2H), 7.62 (dd, J = 2.0, 7.9 Hz, 1H), 7.70 (dt, J = 1.6, 7.5 Hz, 1H), 8.26 (d, J = 8.0 Hz, 1H), 8.41 (d, J = 7.5 Hz, 2H), 8.55 (ddd, J = 1.2, 1.8, 3.8 Hz, 1H) 3 protons signals coincidentally overlapped with solvents; ^{13}C NMR (ODCB-d_4, 100 MHz) δ 52.32, 74.33, 122.61, 122.64, 126.59, 127.66, 127.75, 127.82, 127.85, 127.98, 128.06, 128.54, 129.36, 129.39, 129.62, 130.52, 130.85, 130.90, 131.52, 131.75, 132.05, 132.71, 132.90, 135.15, 135.20, 135.35, 137.25, 137.54, 137.60, 137.72, 137.91, 137.94, 138.19, 138.52, 138.76, 138.79, 138.90, 139.83, 140.00, 140.05, 140.16, 140.35, 140.69, 140.80, 141.06, 141.71, 141.72, 142.38, 144.04, 144.50, 145.15, 145.57, 146.44, 146.70, 146.91, 147.17, 147.20, 147.26, 147.38, 147.50, 147.65, 147.68, 147.70, 147.75, 147.88, 148.03, 148.42, 148.45, 148.50, 148.54, 148.92, 149.04, 149.09, 150.21, 164.01, 166.30, 185.43, 193.66; FT-IR ν (cm^{-1}) (C=O) 1713, 1746. UV-vis ($CHCl_3$, 4.89×10^{-5} M) λ_{max} (ε) 227 (11300), 258 (12300), 319 (4560), 442 (548). HRMS (FAB-positive mode) calcd for $C_{80}H_{15}O_2N_2Se$ ($M + H^+$): 1115.0299; found: 1115.0325.

Synthesis of H_2@3. To a 100 mg fine powder of compound **3** wrapped by aluminum foil was applied high pressure of hydrogen gas (760 atm) in an autoclave at 190 ^{o}C for 8 h. The powder was found to incorporate 100% hydrogen by ^{1}H NMR. Spectral data follow.

^{77}Se NMR (ODCB-d_4, 75.5 MHz): δ 195.7; ^{1}H NMR (ODCB-d_4, 300 MHz) δ –7.10 (s, 2H), 6.78 (t, J = 7.2 Hz, 1H), 7.62 (d, J = 7.2 Hz, 1H), 7.70 (dt, J = 1.5, 7.5 Hz, 1H), 8.26 (d, J = 7.8 Hz, 1H), 8.41 (d, J = 7.2 Hz, 2H), 8.55 (ddd, J = 3.0 Hz, 1H); 3 protons signals coincidentally overlap with solvents; ^{13}C NMR (ODCB-d_4, 75 MHz) δ52.33, 74.34, 122.63, (126–134, signals overlapped with ODCB-d_4), 135.34, 135.38, 135.40, 137.26, 137.66, 137.85, 137.99, 138.27, 138.59, 138.66, 138.80, 138.97, 139.91, 140.08, 140.15, 140.35, 140.81, 140.93, 141.21, 141.83, 141.85, 142.44, 144.08, 144.50, 145.19, 145.51, 146.39, 146.77, 146.97, 147.23, 147.26, 147.33, 147.43, 147.52, 147.54, 147.71, 147.81, 147.92, 148.09, 148.10, 148.51, 148.57, 148.62, 148.88, 149.03, 149.13, 150.19, 164.00, 166.33, 185.46, 193.63; FT-IR ν (cm^{-1}) (C=O) 1708, 1745. MALDI-TOF MS calcd for $C_{80}H_{16}O_2N_2Se$ (M^+): 1116.04; found: 1116.06. UV-vis ($CHCl_3$, 6.67×10^{-5} M) λ_{max} (ε) 227 (10300), 258 (11500), 318 (4360), 438 (588).

Figure S1. MALDI-TOF mass spectrum of compound **3** (terthiophene as matrix)

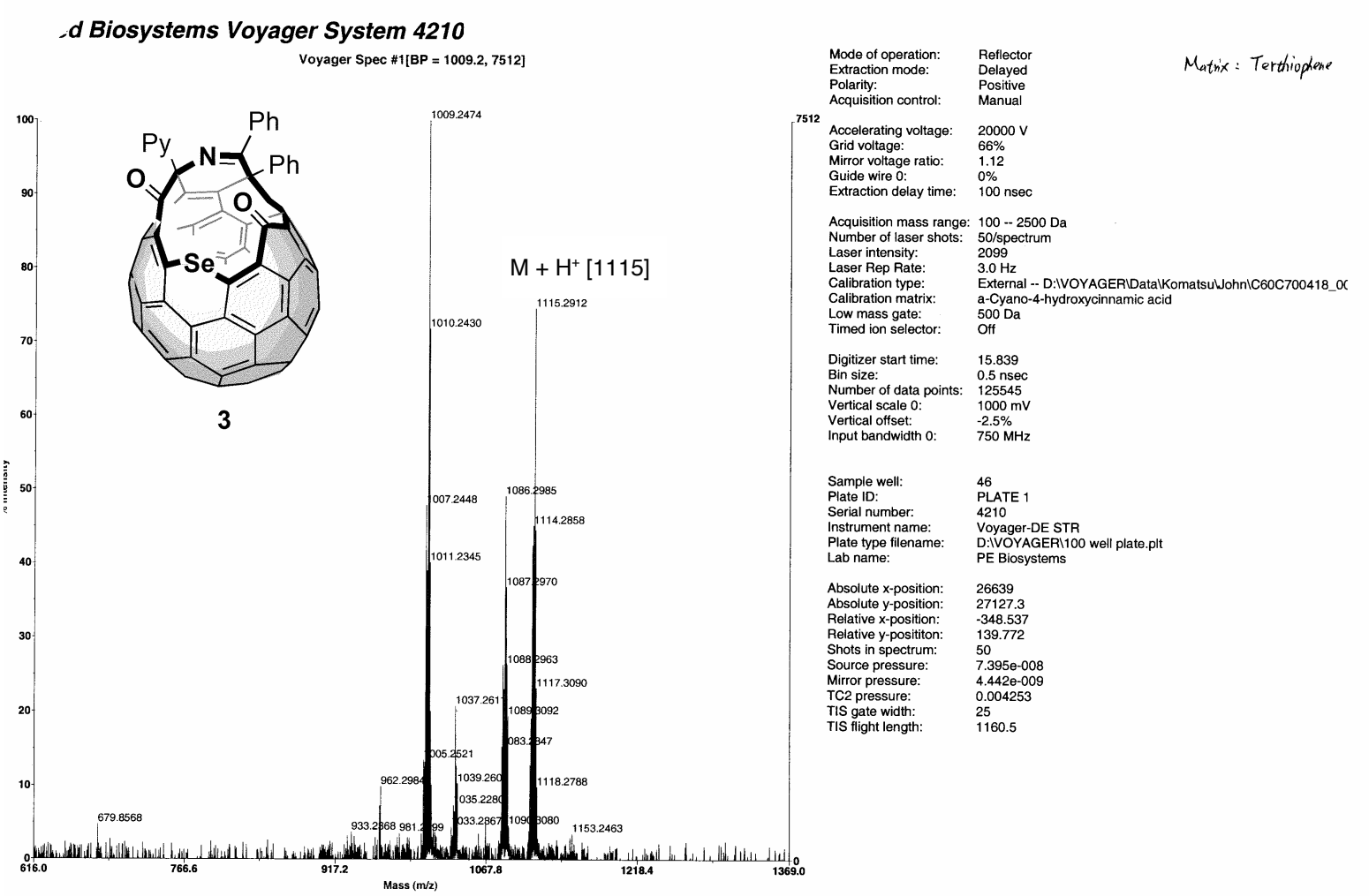


Figure S2. ^{77}Se NMR spectrum of compound **3** (75.5 MHz, ODCB-d_4)

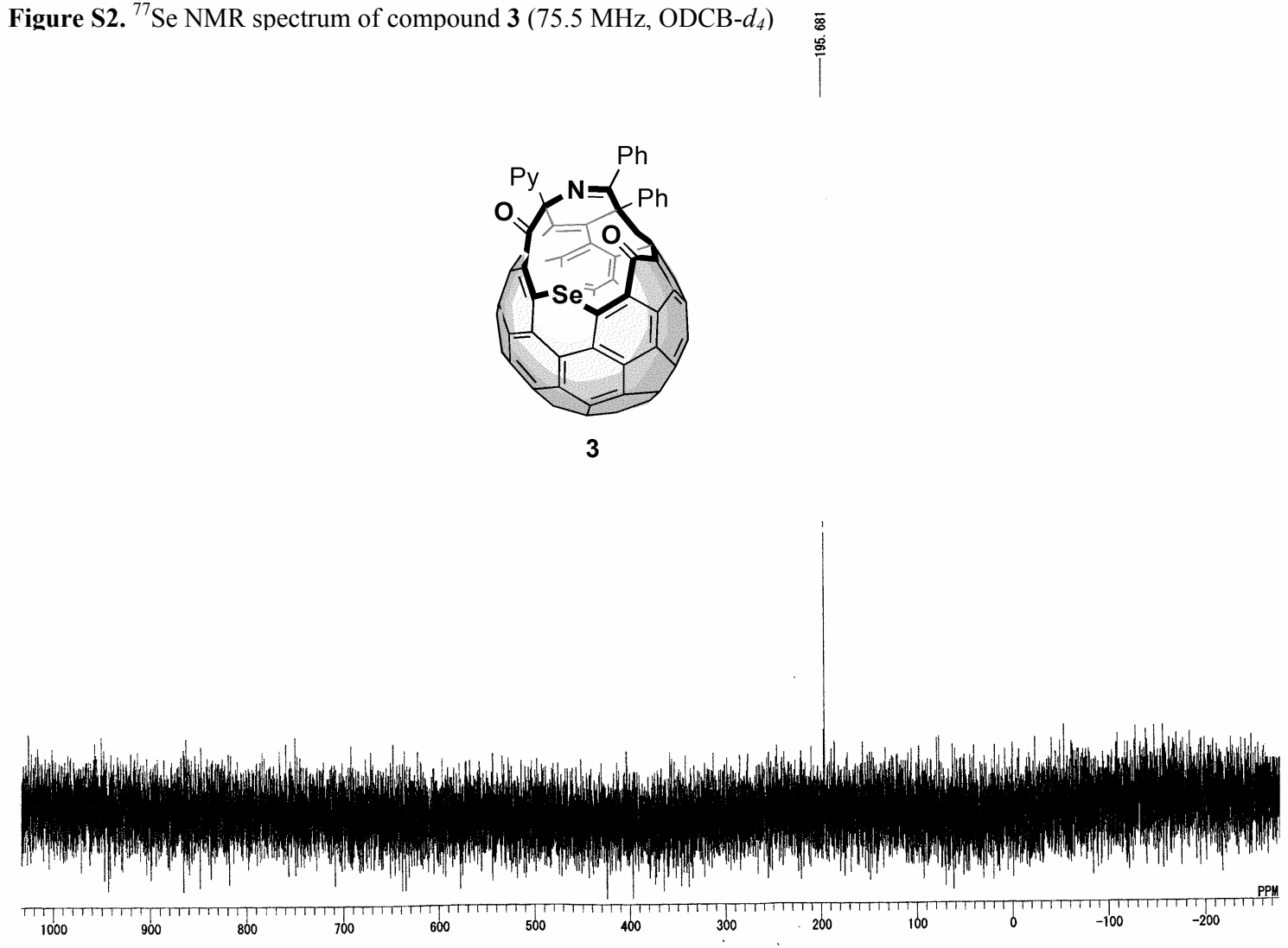


Figure S3. ^{1}H NMR spectrum of compound **3** (400 MHz, ODCB-d_4)

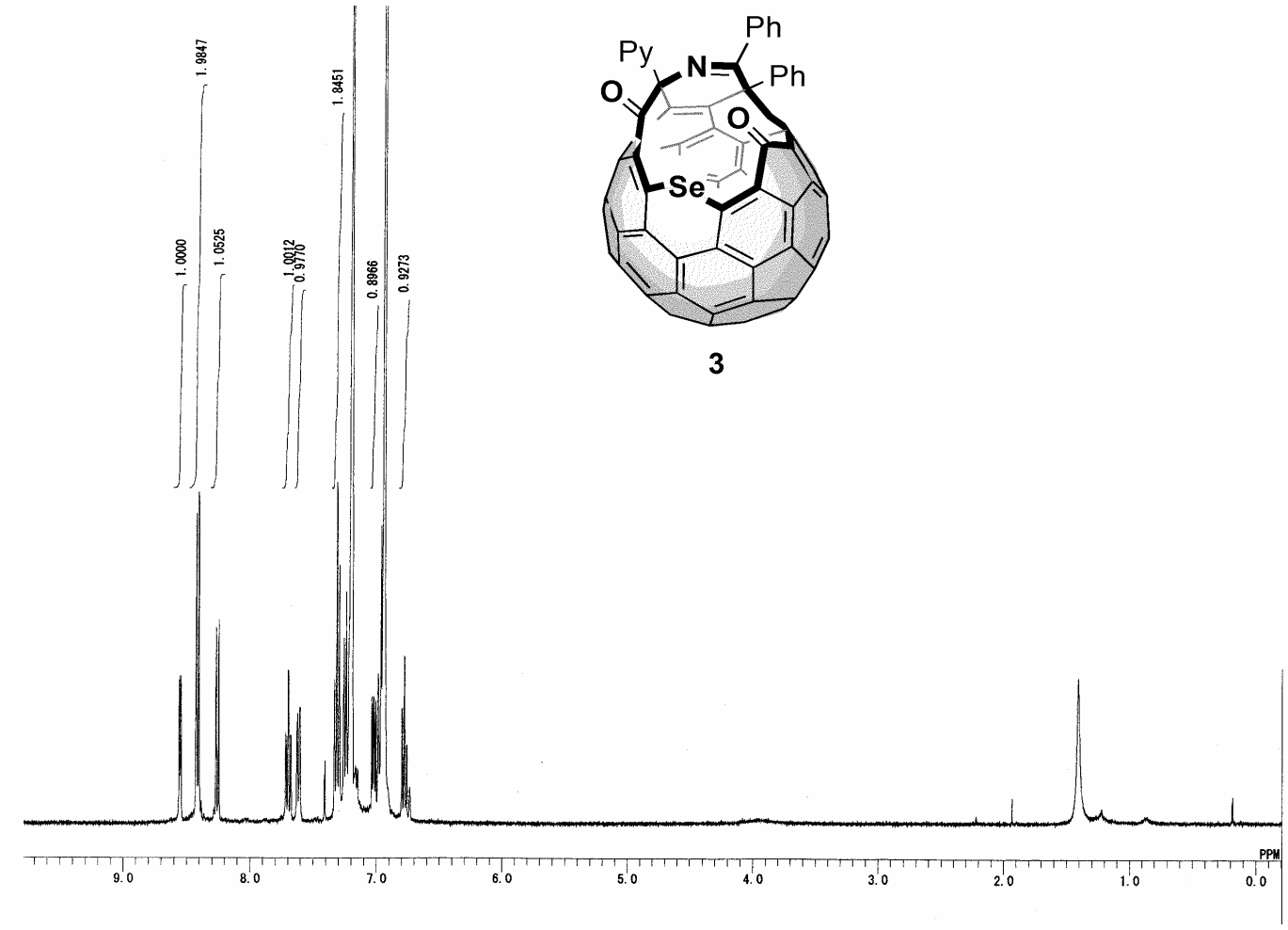


Figure S4. ^{13}C NMR spectrum of compound **3** (100 MHz, ODCB-d_4)

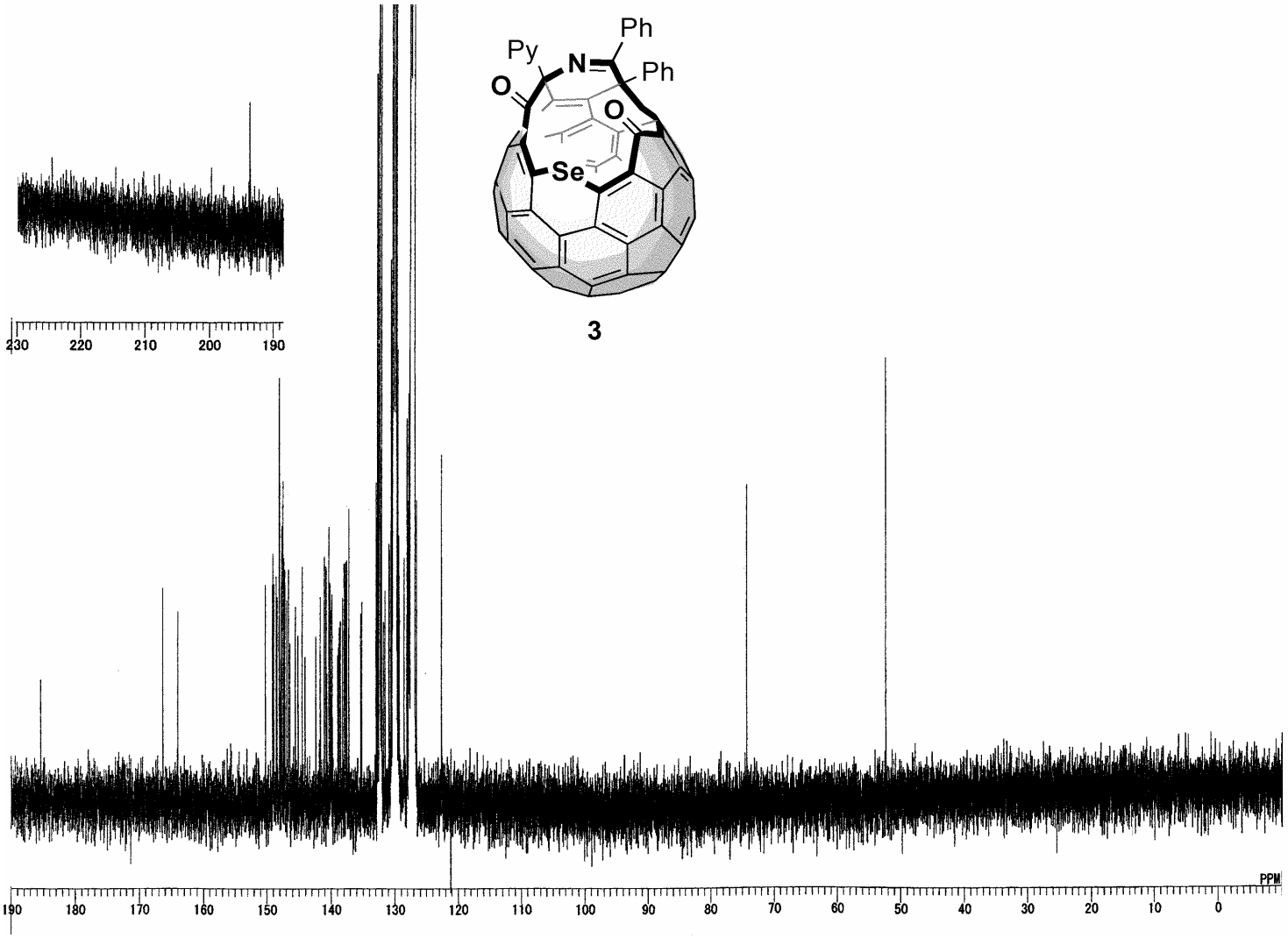


Figure S5. IR spectrum of compound **3** (KBr)

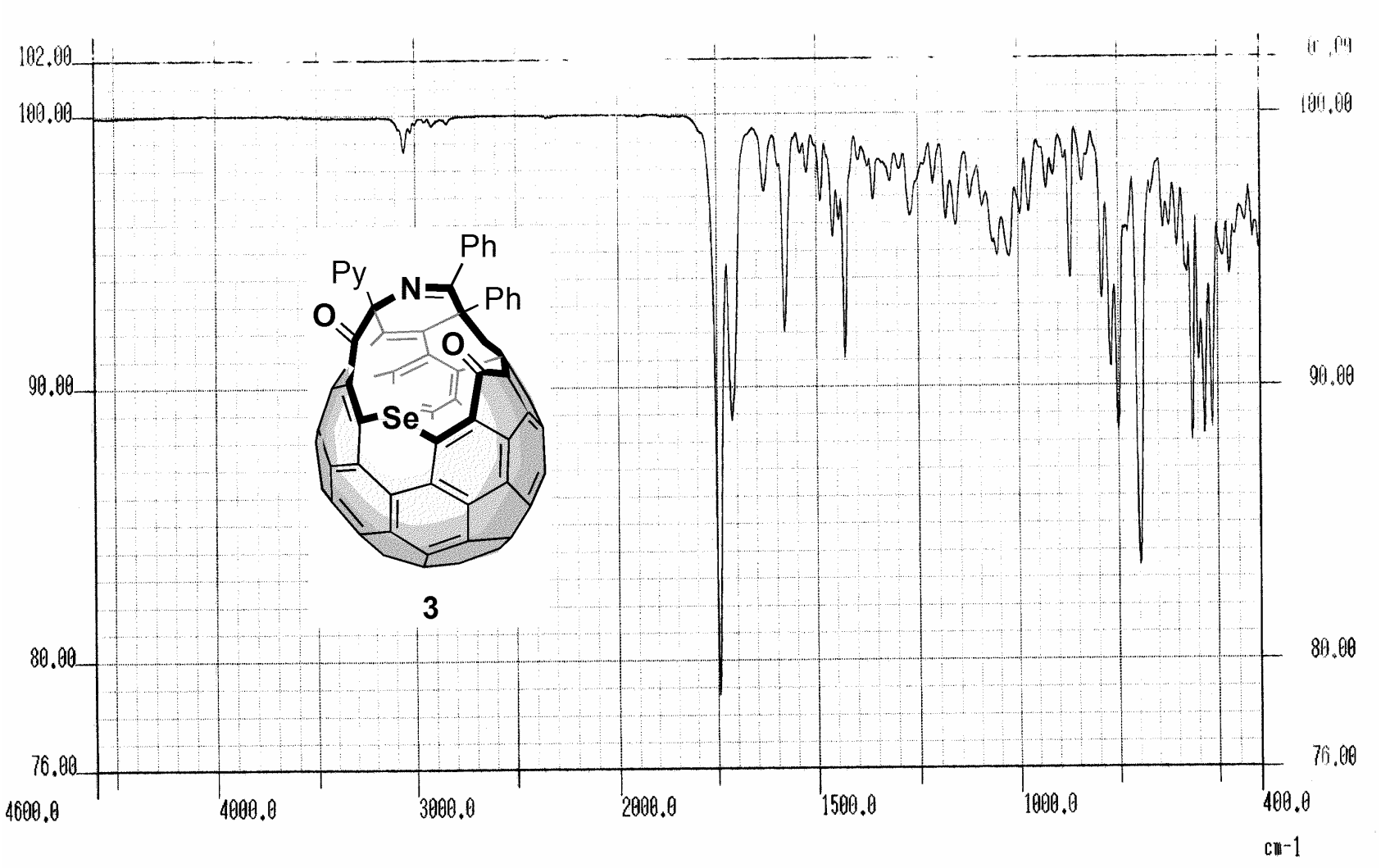


Figure S6. Uv-vis spectrum of compound **3** (4.89×10^{-5} M)

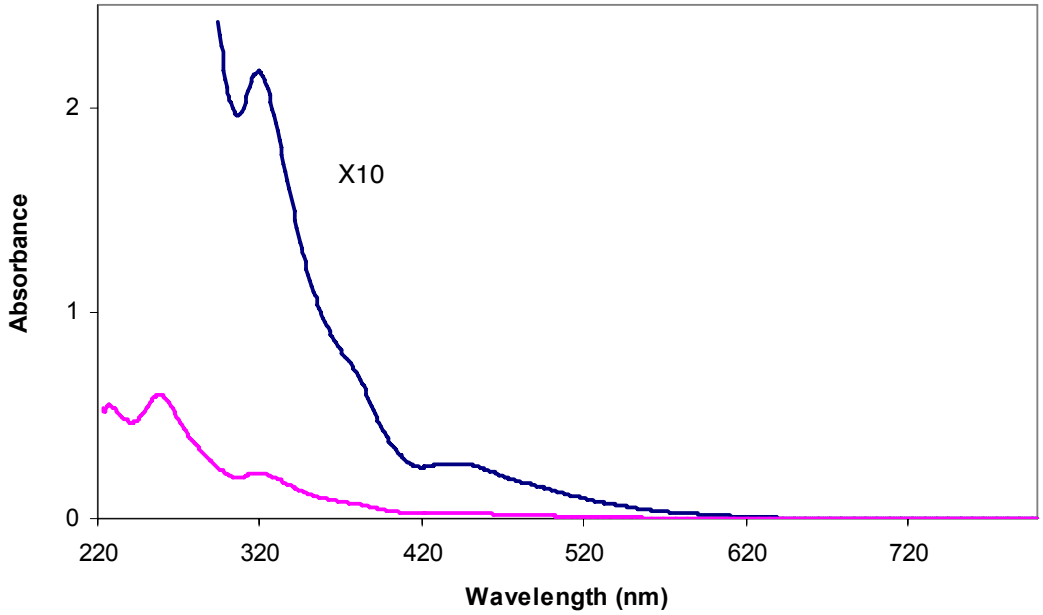


Figure S7. Uv-vis spectrum of compound H_2@**3** (6.67×10^{-5} M)

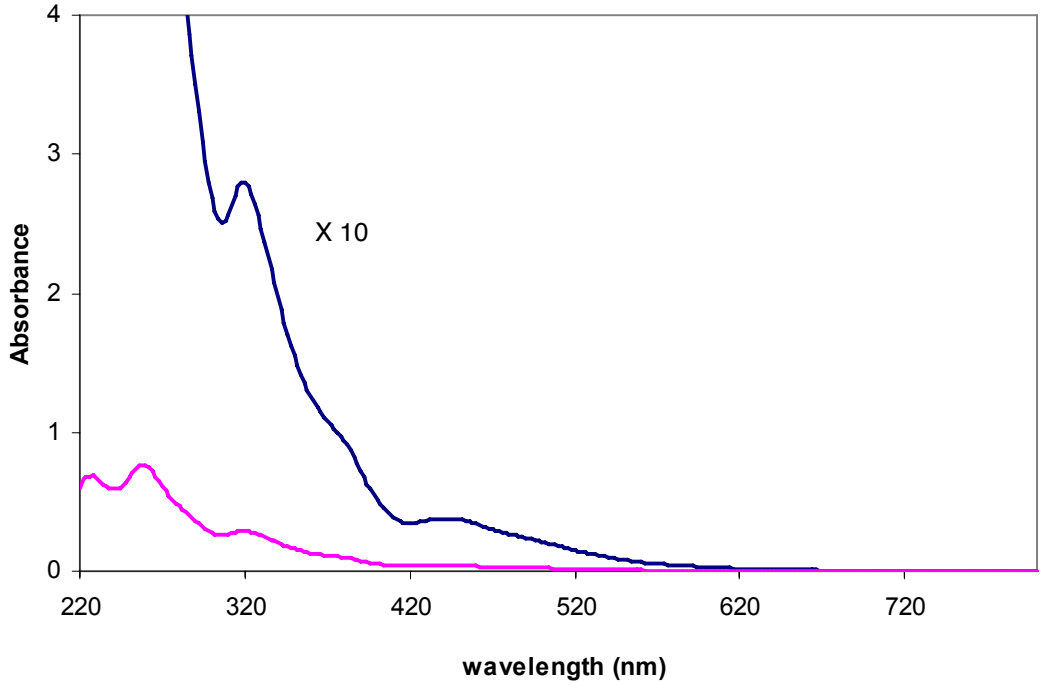


Figure S8. MALDI-TOF mass spectrum of compound H_2@**3** (dithranol as matrix)

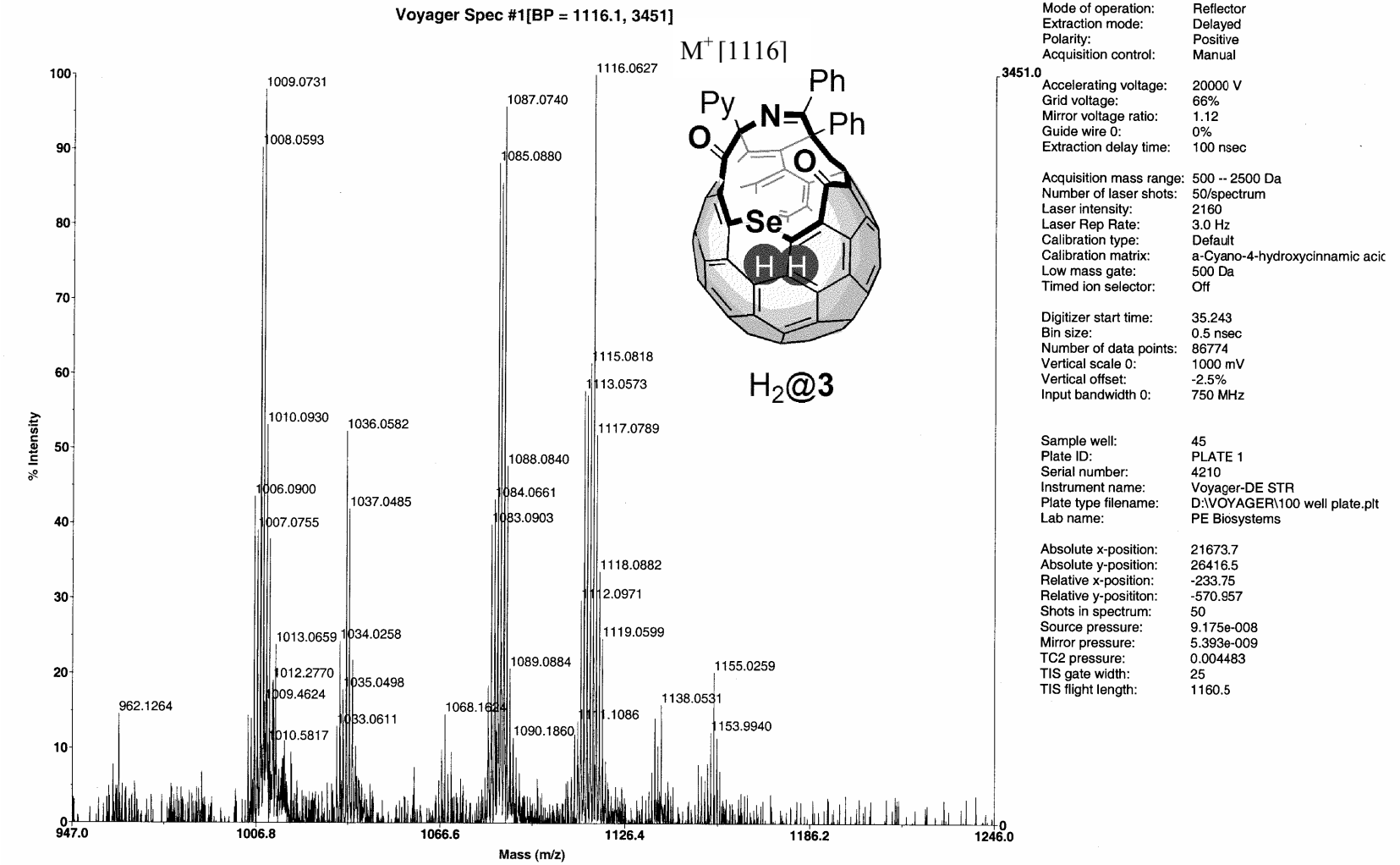


Figure S9. ^{77}Se NMR spectrum of compound H_2@**3** (75.5 MHz, ODCB-d_4)

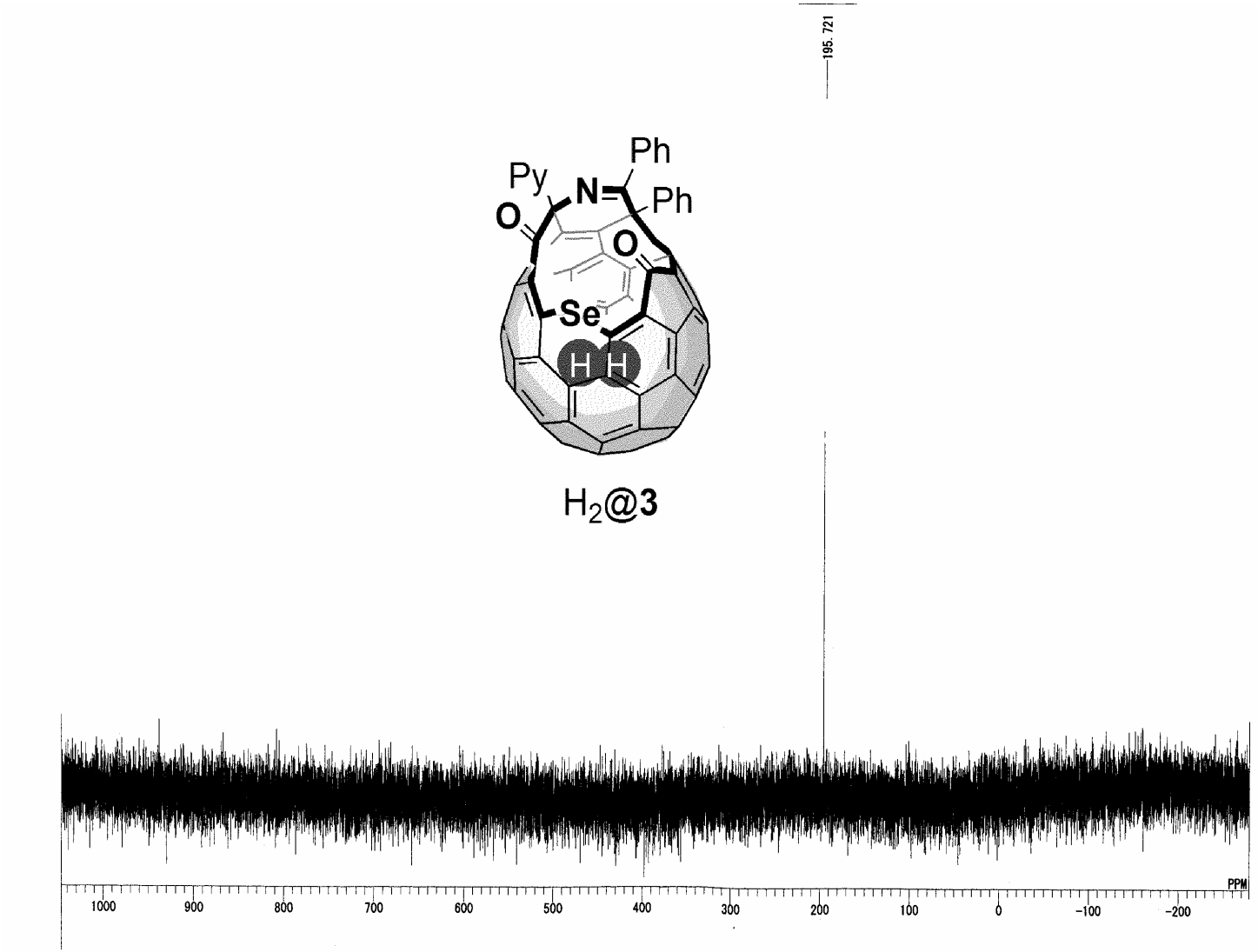


Figure S10. ^{13}C NMR spectrum of compound H_2*@*$\mathbf{3}$ (75 MHz, ODCB-d_4)

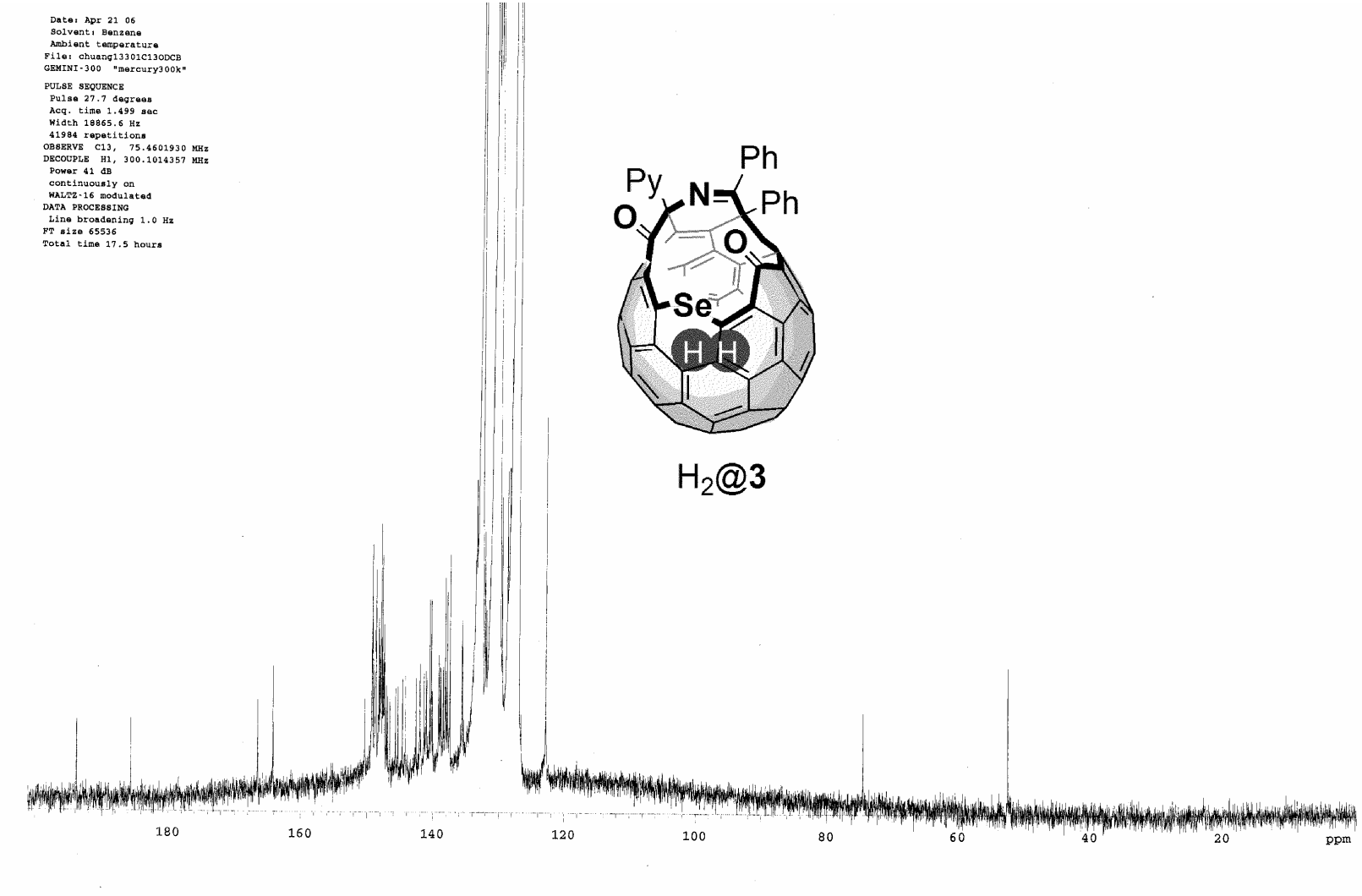


Figure S11. ^{1}H NMR spectrum of compound H_2@**3** (300 MHz, ODCB-d_4)

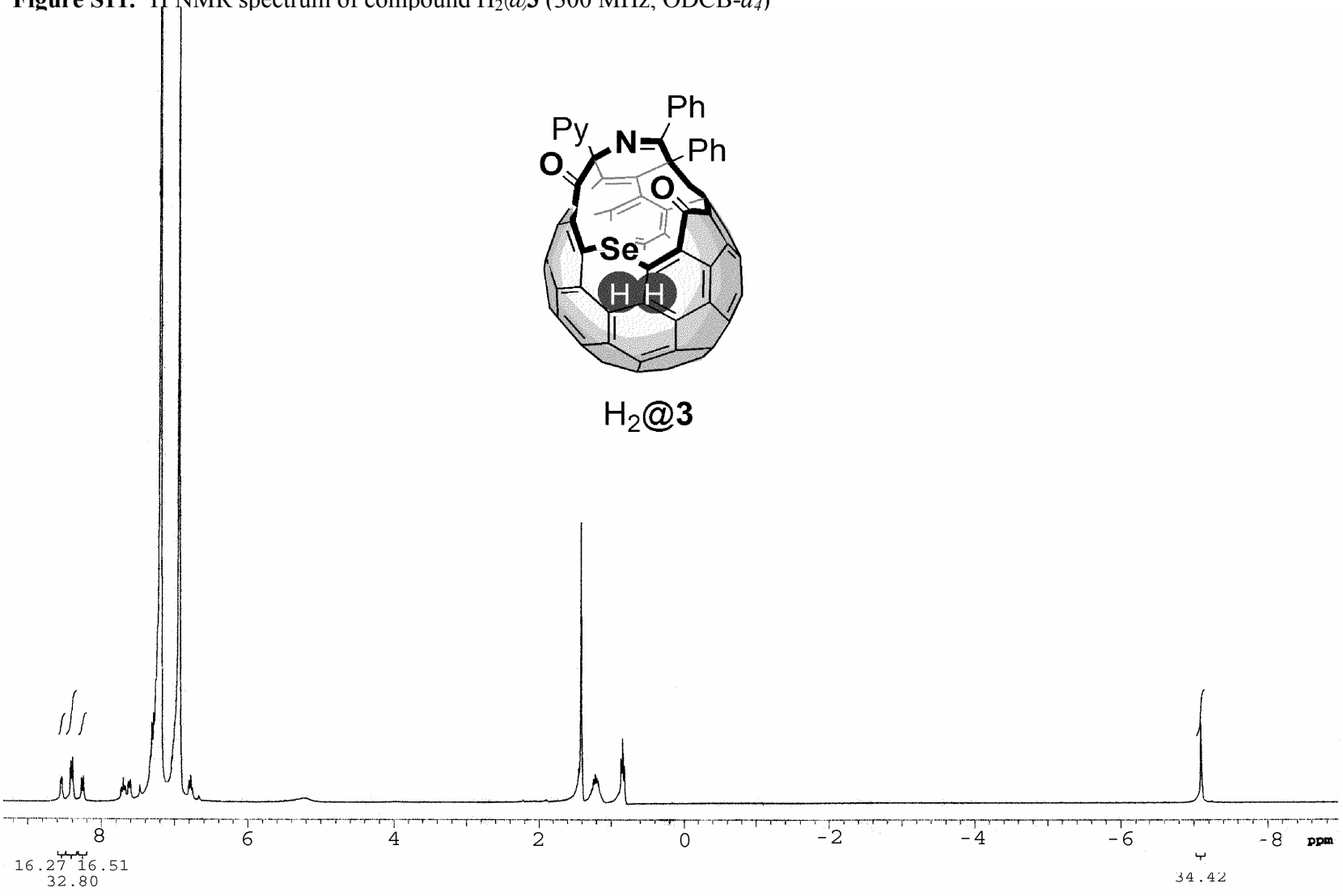
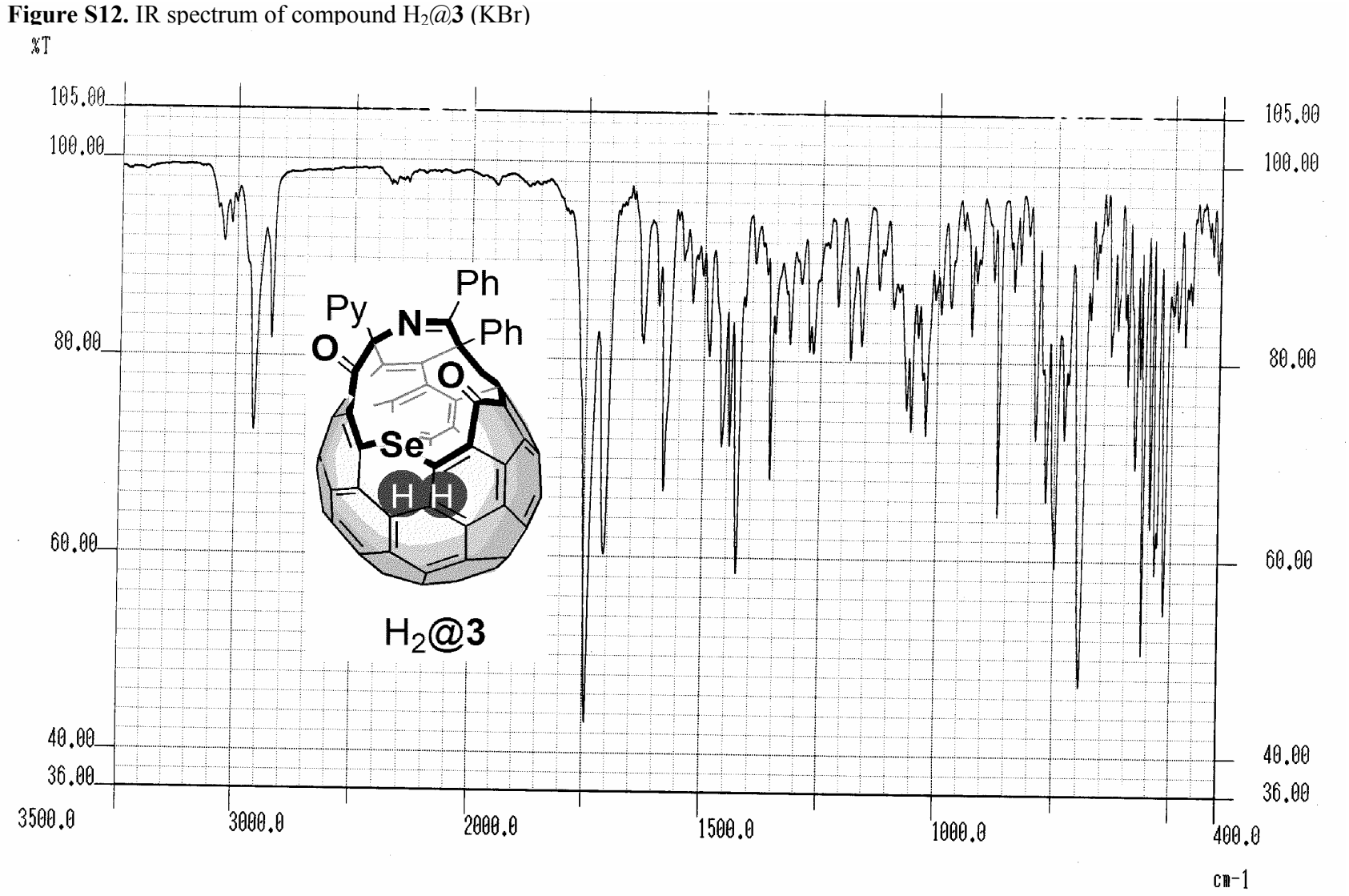


Figure S12. IR spectrum of compound H_2@**3** (KBr)



Kinetic data of H_2 release measurement

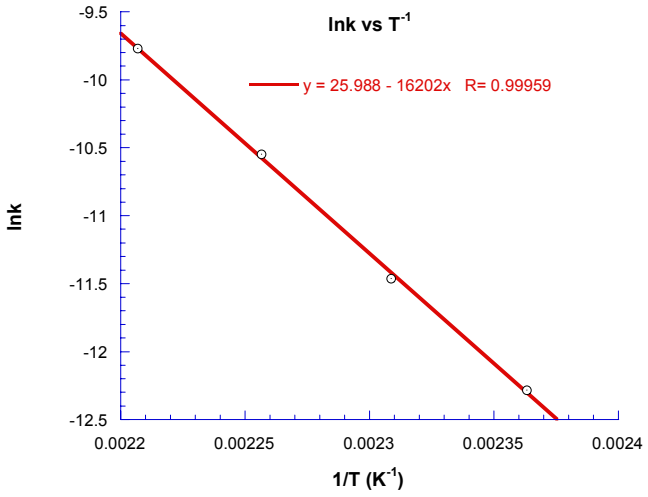
The rate of hydrogen release was measured at four temperatures, 150, 160, 170, and 180 ^{o}C. The nmr sample was prepared by dissolving 4 mg of H_2@**3** in 0.5 mL of ODCB-d_4 and treated with FPT (freeze-pump-thaw) process until no gas evolution occurred. NMR measurement was conducted at appropriate time interval at each temperature and hydrogen content was calculated and plotted against time. The rate constant was extracted from the fitted exponential decay plot.

Temperature (^{o}C)	Half-life (h)	Rate constant ($\times 10^{-6}$) (s^{-1})
150±0.5	41.6	4.63±0.27
160±0.3	18.3	10.5±0.04
170±0.3	7.3	26.2±0.35
180±0.3	3.4	57.2±4.75

	$t_{1/2}$[a]	Ea[c]	A	$\Delta G^{\ddagger}$ (25 ^{o}C)[c]	$\Delta H^{\ddagger}$ (25 ^{o}C)[c]	$\Delta S^{\ddagger}$ (25 ^{o}C)[d]
H_2@**2** [b]	53.9±0.56	34.2±0.58	$10^{11.8\pm0.3}$	35.6±0.59	33.4±0.59	–7.5±1.3
H_2@**3**	18.3±0.56	32.4±0.67	$10^{11.3\pm0.3}$	34.4±0.66	31.5±0.67	–9.6±1.5

[a] Half-life (h) at 160 ^{o}C. [b] Ref. 10 in context. Error limits were re-examined in this study for consistency. [c] kcal·mol^{-1}. [d] cal·K^{-1}·mol^{-1}.

Arrhenius plot



Optimized geometry of compound **2**
(B3LYP/3-21G)

Nimag Frequency = 0
0 1
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Single point energy of compound **2**
(B3LYP/6-31G**//B3LYP/3-21G)
E = -3714.87687242 hartrees

Optimized geometry of compound H_2@**2**
(B3LYP/3-21G)

Nimag Frequency = 0
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C 0 -3.31008 -0.64179 -3.29159
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C 0 3.5648 -0.6162 0.29437
C 0 3.81965 2.85811 -0.37571
C 0 4.45828 -1.61326 0.97165
C 0 3.21297 -1.79536 -1.88473
C 0 5.1661 -1.16076 2.1041
C 0 6.00924 -2.01419 2.80463
C 0 6.15982 -3.34489 2.39888
C 0 5.45779 -3.80657 1.28676
C 0 4.61354 -2.94965 0.5762
C 0 4.21705 -1.0605 -2.5317
C 0 4.93068 -1.61007 -3.59584
C 0 4.65324 -2.90761 -4.03159
C 0 3.65614 -3.64577 -3.39377
C 0 2.93841 -3.09404 -2.32953
N 0 3.19178 3.87261 -0.98747
C 0 3.92562 4.90494 -1.45086
C 0 5.31187 4.95898 -1.31226
C 0 5.95604 3.90415 -0.66039
C 0 5.20122 2.8342 -0.17824
O 0 2.91166 2.45909 2.50958
O 0 2.41774 -0.56394 2.72074
S 0 0.51136 1.58696 3.92741
C 0 1.39965 -1.19186 2.47416
H 0 5.00481 -0.14175 2.42479
H 0 6.53853 -1.64918 3.6772
H 0 6.81341 -4.01289 2.94814
H 0 5.56916 -4.83402 0.96027
H 0 4.11153 -3.32103 -0.30146
H 0 4.44252 -0.0544 -2.19763
H 0 5.70306 -1.02537 -4.08148
H 0 5.20791 -3.33733 -4.85716
H 0 3.43073 -4.65373 -3.72228
H 0 2.1699 -3.6823 -1.84752
H 0 3.38251 5.70464 -1.94122
H 0 5.86775 5.8038 -1.69812
H 0 7.0311 3.91541 -0.52614
H 0 5.64194 1.99915 0.34442
H 0 -1.6712 -0.32982 -0.20698
H 0 -1.9515 -0.05113 0.4249

Single point energy of compound H_2@**2**
(B3LYP/6-31G**//B3LYP/3-21G)
E = -3716.05312482 hartrees

Transition state structure of H_2-**2** (B3LYP/3-21G)
Nimag Frequency =1

0 1
C 0 -3.26039 -0.46545 -3.38421
C 0 -1.82033 -0.30985 -3.5445
C 0 -1.24499 0.93671 -3.41256
C 0 -2.06096 2.09787 -3.07541
C 0 -3.42315 1.93909 -2.84568
C 0 -4.04056 0.62932 -3.01576
C 0 -1.1569 -1.47663 -2.97537
C 0 0.03174 1.06085 -2.75073
C 0 -1.258 2.94254 -2.20677
C 0 -4.036 2.57795 -1.68239
C 0 -5.05886 0.46804 -1.98097
C 0 -3.50069 -1.77024 -2.79143
C 0 -3.24889 3.33395 -0.82142
C 0 -1.83959 3.5495 -1.1017
C 0 -3.37216 3.14676 0.61833
C 0 -1.11521 3.55103 0.15599
C 0 0.04101 -1.35983 -2.2396
C 0 0.05379 2.34119 -2.06303
C 0 -2.05844 3.22447 1.21
C 0 0.81547 2.48442 -0.91352
C 0 0.66436 -0.04164 -2.16401
C 0 -5.03048 1.6614 -1.13878
C 0 -5.2901 -0.78105 -1.4151
C 0 0.28002 -2.27926 -1.10976
C 0 -4.5116 -1.93809 -1.8482
C 0 -2.20532 -2.40601 -2.58529
C 0 -5.5051 -0.9058 0.02361
C 0 -4.29381 -2.80015 -0.69377
C 0 -2.00446 -3.23697 -1.50558
C 0 0.19993 3.10903 0.25214
C 0 -5.17782 1.53028 0.24114
C 0 1.66943 0.2181 -1.15724
C 0 -4.91251 -2.16247 0.46521
C 0 -3.08188 -3.46986 -0.54459
C 0 -0.74393 -3.19005 -0.79195
C 0 -1.02828 -3.51237 0.58989
C 0 1.28455 -1.91793 -0.07851
C 0 1.80059 1.46969 -0.62452
C 0 2.16511 2.53939 1.65655
C 0 -2.47251 -3.60754 0.76482
C 0 -3.06877 -3.00393 1.87322
C 0 -2.23411 -2.30241 2.83764
C 0 -4.28963 -2.23732 1.70636
C 0 -4.28954 2.26067 1.13663
C 0 -5.41955 0.22633 0.8307
C 0 -4.68301 0.16645 2.08718
C 0 0.96989 -2.21782 1.24063
C 0 0.67464 2.69445 1.55431
C 0 -0.24157 2.3475 2.53081
C 0 -0.24672 -2.92156 1.55072
C 0 -0.86551 -2.31841 2.71399
C 0 -4.15815 -1.03001 2.52121
C 0 -2.86635 -1.03787 3.16509
C 0 -0.04289 -1.24215 3.18621
C 0 -3.91261 1.39251 2.24672
C 0 -1.66536 2.41481 2.2875
C 0 -0.65197 -0.05928 3.55247
C 0 -2.61338 1.40175 2.80382
C 0 -2.0872 0.1221 3.33427
C 0 2.42815 -0.99551 -0.60683
C 0 2.83347 1.80961 0.40338
N 0 3.64259 0.65808 0.86902
C 0 3.4933 -0.54807 0.43516
C 0 3.89226 2.7467 -0.22673
C 0 4.50566 -1.53997 0.91899
C 0 3.20514 -1.61776 -1.79785
C 0 5.73946 -1.04144 1.37266
C 0 6.73081 -1.9031 1.83186
C 0 6.50595 -3.282 1.8549
C 0 5.28011 -3.78714 1.41818
C 0 4.28834 -2.92517 0.95167
C 0 3.98522 -0.75018 -2.57794
C 0 4.72798 -1.2425 -3.65022
C 0 4.69708 -2.60385 -3.96282
C 0 3.91469 -3.46781 -3.19672
C 0 3.17299 -2.97719 -2.11912
N 0 3.90045 2.82158 -1.56822
C 0 4.84435 3.5854 -2.16381
C 0 5.81018 4.28491 -1.44511
C 0 5.80686 4.18047 -0.05084
C 0 4.8386 3.39524 0.57215
O 0 2.82204 2.9762 2.5992
O 0 2.45492 -1.66522 3.20357
S 0 0.25512 1.4748 4.0915
C 0 1.37594 -1.65264 2.64791
H 0 5.89449 0.02863 1.35512
H 0 7.67869 -1.50097 2.17018
H 0 7.27676 -3.95551 2.21119
H 0 5.09199 -4.85407 1.44455
H 0 3.34039 -3.33526 0.63858
H 0 3.9909 0.31252 -2.3564
H 0 5.32546 -0.5614 -4.24499
H 0 5.27275 -2.98536 -4.79792
H 0 3.87769 -4.52458 -3.43441
H 0 2.56311 -3.65786 -1.54025
H 0 4.81759 3.62633 -3.24649
H 0 6.54717 4.88709 -1.96089
H 0 6.54844 4.70193 0.54229
H 0 4.78331 3.28822 1.64459
H 0 1.67007 0.58822 2.4294
H 0 2.39537 0.47451 2.45165

Single point energy of compound H_2-**2** (B3LYP/6-31G**//B3LYP/3-21G)
E = -3716.0070072 hartrees

Optimized geometry of compound **3**
(B3LYP/3-21G)
Nimag Frequency = 0
0 1

C	0	3.388273	1.678854	-3.008919
C	0	1.955206	1.637670	-3.273241
C	0	1.353529	0.446010	-3.621463
C	0	2.131799	-0.785913	-3.683867
C	0	3.483832	-0.764290	-3.357434
C	0	4.130714	0.499187	-3.024686
C	0	1.283280	2.545401	-2.351126
C	0	0.040321	0.137174	-3.105546
C	0	1.271246	-1.854369	-3.204284
C	0	4.027561	-1.793691	-2.475801
C	0	5.101463	0.248234	-1.962496
C	0	3.619492	2.676007	-1.977722
C	0	3.182281	-2.775026	-1.967636
C	0	1.784919	-2.826852	-2.357892
C	0	3.241592	-3.112341	-0.551418
C	0	0.999314	-3.235713	-1.205257
C	0	0.045811	2.215540	-1.762735
C	0	-0.039501	-1.301113	-2.918860
C	0	1.899063	-3.337622	-0.072715
C	0	-0.862029	-1.816251	-1.926048
C	0	-0.613397	0.988221	-2.203762
C	0	5.012612	-1.165355	-1.604135
C	0	5.326024	1.205290	-0.978925
C	0	-0.226743	2.664792	-0.380978
C	0	4.586376	2.464145	-0.997895
C	0	2.325595	3.234673	-1.606349
C	0	5.479757	0.802465	0.415671
C	0	4.328415	2.862615	0.380182
C	0	2.086919	3.625709	-0.307265
C	0	-0.309781	-2.810965	-1.009622
C	0	5.099732	-1.538922	-0.264441
C	0	-1.676768	0.421485	-1.407516
C	0	4.887977	1.836959	1.255706
C	0	3.118574	3.466951	0.714846
C	0	0.794991	3.357728	0.291662
C	0	1.010482	3.146405	1.705081
C	0	-1.275321	1.979231	0.400962
C	0	-1.848838	-0.935378	-1.353648
C	0	-2.275445	-2.573756	0.533186
C	0	2.449678	3.142836	1.961998
C	0	2.995918	2.174386	2.806020
C	0	2.115823	1.201490	3.433842
C	0	4.214597	1.484546	2.419633
C	0	4.157817	-2.509456	0.279832
C	0	5.339265	-0.540086	0.761039
C	0	4.553759	-0.910609	1.932003
C	0	-1.005802	1.717997	1.743575
C	0	-0.826242	-2.860998	0.335211
C	0	0.043728	-2.939909	1.412246
C	0	0.181603	2.257626	2.351011
C	0	0.751709	1.290103	3.265020
C	0	4.033964	0.071064	2.747379
C	0	2.722873	-0.114660	3.316075
C	0	-0.063035	0.129339	3.290580
C	0	3.755614	-2.089758	1.616986
C	0	1.474979	-2.965219	1.212627
C	0	0.504711	-1.127276	3.285506
C	0	2.438485	-2.264463	2.100322
C	0	1.928369	-1.247772	3.048644
C	0	-2.417585	1.372311	-0.456235
C	0	-2.911902	-1.568751	-0.517587
N	0	-3.754479	-0.639660	0.230845
C	0	-3.520623	0.618744	0.341070
C	0	-3.821983	-2.450387	-1.401492
C	0	-4.413093	1.371604	1.283153
C	0	-3.141094	2.411898	-1.364609
C	0	-5.162156	0.604652	2.198636
C	0	-6.009474	1.215910	3.114139
C	0	-6.122491	2.610408	3.147166
C	0	-5.377902	3.380064	2.255002
C	0	-4.529826	2.768093	1.328664
C	0	-4.157628	1.926460	-2.200080
C	0	-4.855145	2.784632	-3.049046
C	0	-4.548442	4.146823	-3.076932
C	0	-3.538329	4.638175	-2.249900
C	0	-2.836784	3.777823	-1.401365
N	0	-3.201133	-3.232145	-2.296708
C	0	-3.944854	-4.044303	-3.075057
C	0	-5.334538	-4.105459	-2.979603
C	0	-5.971608	-3.298183	-2.033828
C	0	-5.206399	-2.456671	-1.224905
O	0	-2.942023	-3.031343	1.456910
O	0	-2.422395	-0.159031	2.670713
Se	0	-0.607291	-2.689906	3.205341
C	0	-1.387869	0.489961	2.626445
H	0	-5.030111	-0.467622	2.183462
H	0	-6.571871	0.608827	3.814087
H	0	-6.779961	3.088574	3.864234
H	0	-5.458761	4.460775	2.268562
H	0	-3.994772	3.383874	0.625221
H	0	-4.405459	0.871497	-2.183381
H	0	-5.637318	2.388633	-3.685986
H	0	-5.090100	4.815835	-3.734909
H	0	-3.289498	5.693015	-2.262564
H	0	-2.056948	4.178133	-0.768641
H	0	-3.407212	-4.659297	-3.787552
H	0	-5.898547	-4.768962	-3.622482
H	0	-7.049247	-3.325018	-1.924638
H	0	-5.642171	-1.822837	-0.467702

Single point energy of compound **3**
(B3LYP/6-31G**//B3LYP/3-21G)
E = -5716.07742677 hartrees

Optimized geometry of compound H_2@**3**
(B3LYP/3-21G)
Nimag frequency =0
0 1

C	0	3.382003	1.696274	-2.999499
C	0	1.948982	1.656603	-3.264188
C	0	1.347496	0.466734	-3.618533
C	0	2.125781	-0.764841	-3.688875
C	0	3.478200	-0.745108	-3.363050
C	0	4.124244	0.516685	-3.021611
C	0	1.276796	2.559046	-2.336959
C	0	0.034159	0.155162	-3.104556
C	0	1.265212	-1.836111	-3.215238
C	0	4.021650	-1.779275	-2.486633
C	0	5.095258	0.259750	-1.961072
C	0	3.612758	2.687416	-1.962324
C	0	3.176381	-2.763533	-1.983873
C	0	1.778965	-2.813155	-2.374128
C	0	3.236119	-3.109511	-0.569617
C	0	0.993507	-3.229139	-1.223789
C	0	0.038400	2.227078	-1.751184
C	0	-0.045446	-1.284206	-2.926025
C	0	1.893529	-3.338310	-0.092039
C	0	-0.867640	-1.804725	-1.935866
C	0	-0.620701	1.001777	-2.199271
C	0	5.006453	-1.155876	-1.611054
C	0	5.320642	1.211351	-0.972261
C	0	-0.235402	2.669763	-0.367282
C	0	4.578717	2.469041	-0.983320
C	0	2.318798	3.244195	-1.588212
C	0	5.472845	0.800114	0.420182
C	0	4.321043	2.860327	0.396655
C	0	2.079388	3.627954	-0.286991
C	0	-0.315464	-2.805077	-1.025364
C	0	5.092931	-1.536771	-0.273447
C	0	-1.684103	0.430238	-1.406397
C	0	4.880253	1.829374	1.266076
C	0	3.110831	3.462018	0.734400
C	0	0.786907	3.357583	0.310024
C	0	1.002386	3.136431	1.721957
C	0	-1.284117	1.978636	0.410129
C	0	-1.854713	-0.927137	-1.358811
C	0	-2.280861	-2.576602	0.519070
C	0	2.441468	3.130452	1.979114
C	0	2.987654	2.157117	2.817452
C	0	2.107887	1.180487	3.439495
C	0	4.206574	1.470058	2.427622
C	0	4.152345	-2.511476	0.265337
C	0	5.333569	-0.544465	0.758030
C	0	4.548032	-0.922086	1.927190
C	0	-1.013920	1.707272	1.750518
C	0	-0.831679	-2.863377	0.319331
C	0	0.038359	-2.950798	1.395704
C	0	0.173775	2.242679	2.361128
C	0	0.744329	1.269014	3.267947
C	0	4.026577	0.054829	2.747331
C	0	2.715811	-0.134790	3.315532
C	0	-0.069604	0.107841	3.286053
C	0	3.750349	-2.099796	1.605307
C	0	1.469791	-2.974440	1.195854
C	0	0.498133	-1.148478	3.278078
C	0	2.433143	-2.278202	2.087765
C	0	1.922347	-1.267531	3.042494
C	0	-2.425855	1.375976	-0.450668
C	0	-2.917384	-1.565485	-0.526290
N	0	-3.760576	-0.640839	0.227023
C	0	-3.528281	0.617344	0.342990
C	0	-3.827176	-2.443383	-1.414264
C	0	-4.420603	1.364122	1.290132
C	0	-3.149737	2.419780	-1.353499
C	0	-5.165590	0.591388	2.204091
C	0	-6.011534	1.196596	3.124886
C	0	-6.127398	2.590665	3.164718
C	0	-5.387268	3.365993	2.273757
C	0	-4.540534	2.760135	1.342175
C	0	-4.165651	1.938214	-2.191985
C	0	-4.864190	2.800738	-3.035659
C	0	-4.559073	4.163447	-3.055239
C	0	-3.549545	4.650977	-2.225235
C	0	-2.847080	3.786285	-1.381884
N	0	-3.206688	-3.216976	-2.316698
C	0	-3.950319	-4.026382	-3.098047
C	0	-5.339435	-4.092999	-2.998293
C	0	-5.976115	-3.293940	-2.045275
C	0	-5.211081	-2.455127	-1.233469
O	0	-2.948000	-3.039653	1.439612
O	0	-2.429063	-0.177037	2.666826
Se	0	-0.611704	-2.712323	3.190943
C	0	-1.394805	0.472463	2.625398
H	0	-5.031176	-0.480492	2.183789
H	0	-6.570548	0.585070	3.823678
H	0	-6.783639	3.064120	3.886030
H	0	-5.470521	4.446448	2.292439
H	0	-4.009016	3.380230	0.639887
H	0	-4.412203	0.882861	-2.181659
H	0	-5.645954	2.407753	-3.674965
H	0	-5.101589	4.835805	-3.709086
H	0	-3.302023	5.706180	-2.231447
H	0	-2.067978	4.183780	-0.746411
H	0	-3.413015	-4.634685	-3.816514
H	0	-5.903304	-4.754439	-3.643416
H	0	-7.053282	-3.325216	-1.932624
H	0	-5.646425	-1.827466	-0.470916
H	0	1.698114	0.450922	-0.182608
H	0	1.967016	-0.015406	0.332106

Single point energy of compound H_2@**3**
(B3LYP/6-31G**//B3LYP/3-21G)
E = -5717.25322658 hartrees

Transition state structure of H_2-**3**
(B3LYP/3-21G)
Nimag Frequency = 1
0 1

C	0	-3.34313	-1.28726	-3.2458
C	0	-1.90627	-1.19252	-3.4743
C	0	-1.31789	0.04269	-3.6475
C	0	-2.11469	1.2618	-3.5654
C	0	-3.47085	1.17901	-3.2680
C	0	-4.10295	-0.12587	-3.1167
C	0	-1.23698	-2.20577	-2.6681
C	0	-0.02171	0.29761	-3.0651
C	0	-1.27909	2.27079	-2.9367
C	0	-4.04405	2.07578	-2.2671
C	0	-5.09207	-0.03129	-2.0462
C	0	-3.57743	-2.41775	-2.3637
C	0	-3.22359	2.99539	-1.6227
C	0	-1.82257	3.12036	-1.9831
C	0	-3.30465	3.14083	-0.1743
C	0	-1.06011	3.39201	-0.7772
C	0	-0.01831	-1.93883	-2.0093
C	0	0.03406	1.70105	-2.6975
C	0	-1.97318	3.32586	0.3476
C	0	0.8317	2.09616	-1.6331
C	0	0.62483	-0.6531	-2.2641
C	0	-5.02782	1.32216	-1.5002
C	0	-5.31892	-1.11445	-1.2039
C	0	0.23908	-2.57126	-0.7003
C	0	-4.5628	-2.3512	-1.3809
C	0	-2.28175	-3.00578	-2.0486
C	0	-5.49416	-0.90388	0.2303
C	0	-4.32107	-2.93104	-0.0662
C	0	-2.05827	-3.57111	-0.8130
C	0	0.2528	2.97021	-0.6182
C	0	-5.13541	1.51159	-0.1236
C	0	1.66429	-0.18308	-1.3772
C	0	-4.90175	-2.03598	0.9319
C	0	-3.10983	-3.56512	0.2018
C	0	-0.77904	-3.37701	-0.1602
C	0	-1.02568	-3.37506	1.2643
C	0	1.27793	-2.00296	0.1948
C	0	1.81786	1.15929	-1.1497
C	0	2.25221	2.73122	0.8229
C	0	-2.46565	-3.41026	1.4924
C	0	-3.02739	-2.56315	2.4486
C	0	-2.1613	-1.67466	3.2080
C	0	-4.24473	-1.83512	2.1408
C	0	-4.214	2.41204	0.5575
C	0	-5.37249	0.3812	0.7547
C	0	-4.60056	0.59896	1.9719
C	0	1.00285	-1.99269	1.5585
C	0	0.75996	2.86758	0.7308
C	0	-0.11989	2.77219	1.7937
C	0	-0.21224	-2.59343	2.0461
C	0	-0.79767	-1.73769	3.0573
C	0	-4.07677	-0.47599	2.6534
C	0	-2.76864	-0.35705	3.2496
C	0	0.03905	-0.59422	3.2605
C	0	-3.80939	1.81347	1.8251
C	0	-1.54963	2.77915	1.5674
C	0	-0.53318	0.65511	3.37855
C	0	-2.49473	1.93187	2.33514
C	0	-1.96907	0.7939	3.1297
C	0	2.41577	-1.24758	-0.56175
C	0	2.88215	1.70905	-0.25475
N	0	3.69201	0.68865	0.42171
C	0	3.50012	-0.58429	0.33258
C	0	3.826	2.58816	-1.10485
C	0	4.43966	-1.45095	1.1152
C	0	3.17236	-2.13951	-1.59227
C	0	5.48129	-0.82506	1.82609
C	0	6.38269	-1.57063	2.57622
C	0	6.26134	-2.96227	2.64117
C	0	5.22825	-3.59395	1.94919
C	0	4.32619	-2.84693	1.19108
C	0	4.14884	-1.51524	-2.38258
C	0	4.86671	-2.23824	-3.3338
C	0	4.61924	-3.60104	-3.51387
C	0	3.64789	-4.22913	-2.73541
C	0	2.92798	-3.5036	-1.78229
N	0	3.21778	3.54007	-1.83032
C	0	3.97076	4.35309	-2.59657
C	0	5.35999	4.24458	-2.66384
C	0	5.98585	3.26154	-1.89526
C	0	5.20989	2.41873	-1.09593
O	0	2.95464	3.36011	1.60331
O	0	2.52575	-1.01913	3.33437
Se	0	0.43903	2.3228	3.59011
C	0	1.43879	-1.12696	2.8055
H	0	5.55034	0.25314	1.78831
H	0	7.17614	-1.06852	3.1175
H	0	6.96182	-3.5454	3.22763
H	0	5.12113	-4.6713	1.99616
H	0	3.53965	-3.3613	0.66377
H	0	4.34693	-0.45736	-2.25514
H	0	5.61696	-1.73684	-3.93389
H	0	5.17602	-4.16461	-4.25302
H	0	3.44345	-5.28536	-2.86663
H	0	2.17334	-4.00729	-1.19368
H	0	3.44298	5.109	-3.16662
H	0	5.93159	4.91346	-3.29419
H	0	7.06373	3.15295	-1.91265
H	0	5.65133	1.65838	-0.47013
H	0	2.56051	0.90363	2.10238
H	0	1.83522	1.01635	2.09245

Single point energy of compound H_2-**3**
(B3LYP/6-31G**//B3LYP/3-21G)
E = -5717.20828056 hartrees