Electronic Supplementary Material (ESI) for New Journal of Chemistry.


**Supporting Information**

# Effect of chalcogen atom variation in chalcogenadiazole fused indolo[2,3-*a*]carbazoles

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**Table 1.** Crystallographic data and structure refinement parameters.

| Formula | $C_{26}H_{26}N_4S$ | $C_{26}H_{26}N_4O$ |
|---|---|---|
| Crystal system | Monoclinic | Triclinic |
| space group | C 1 2/c 1 | P $\bar{1}$ |
| a [Å] | 20.8253(6) | 8.5102(12) |
| b [Å] | 14.6218(5) | 11.3944(18) |
| c [Å] | 16.0280(6) | 11.7116(19) |
| α [deg] | 90 | 97.936(13) |
| β [deg] | 109.450(4) | 96.991(13) |
| γ [deg] | 90 | 110.090(14) |
| V [Å3] | 4602.1(3) | 1038.7(3) |
| Z | 8 | 2 |
| λ [Å] | 0.71073 | 0.71073 |
| ρcalcd | 1.354 | 1.313 |
| F[000] | 1976 | 436 |
| μ [mm−1] | 0.280 | 0.082 |
| θ [deg] | 2.39-27.79 | 2.57-26.94 |
| index ranges | $-19 \le h \le 26$<br>$-18 \le k \le 13$<br>$-20 \le l \le 20$ | $-11 \le h \le 10$<br>$-14 \le k \le 14$<br>$-6 \le l \le 15$ |
| T [K] | 100.00(10) | 100.01(10) |
| R1 | 0.0522 | 0.0960 |
| wR2 | 0.1151 | 0.2506 |
| Rmerge | 0.0617 | 0.1150 |
| parameters | 296 | 282 |
| GOF | 1.042 | 1.133 |
| reflns total | 9335 | 6766 |
| unique reflns | 4691 | 3591 |
| obsd reflns | 4004 | 2855 |
| CCDC No. | 1577362 | 1577361 |

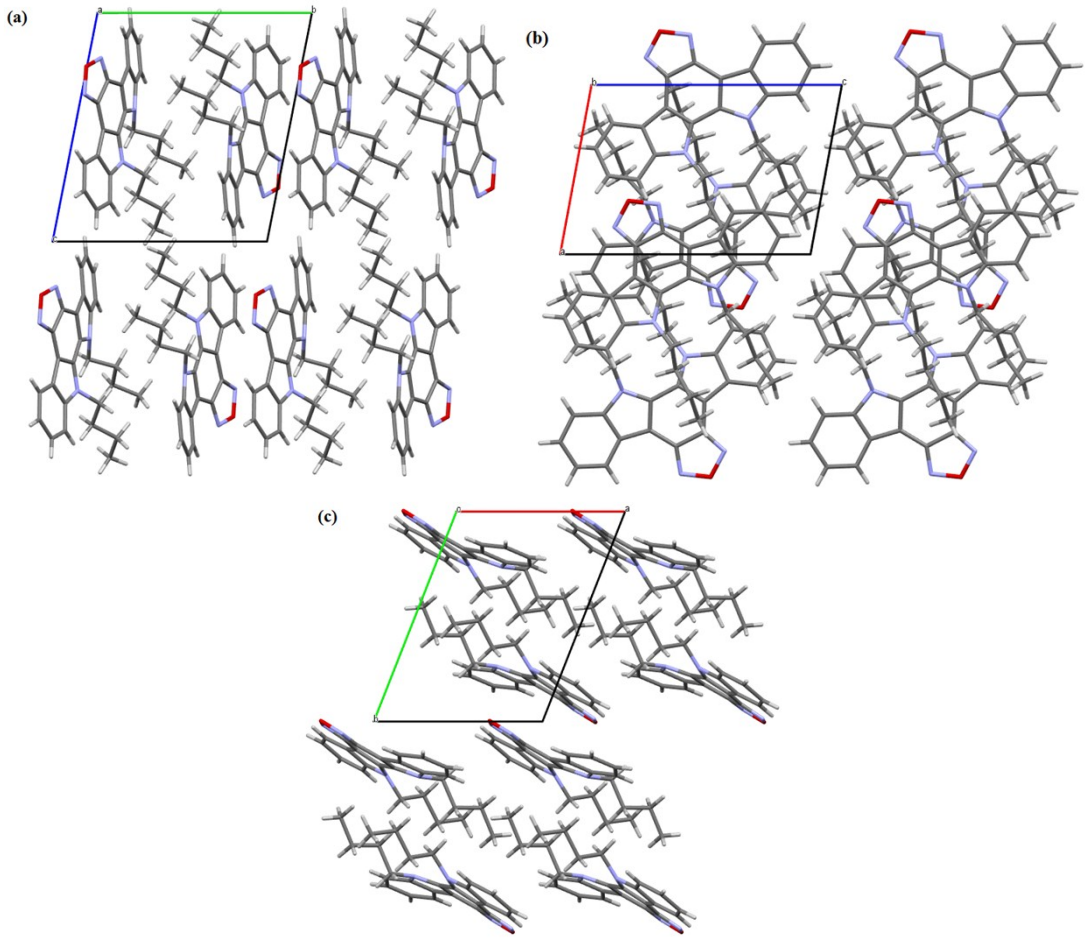


**Figure S1.** Packing diagram of compound **1** along (a) a-axis, (b) b-axis and (c) c-axis.

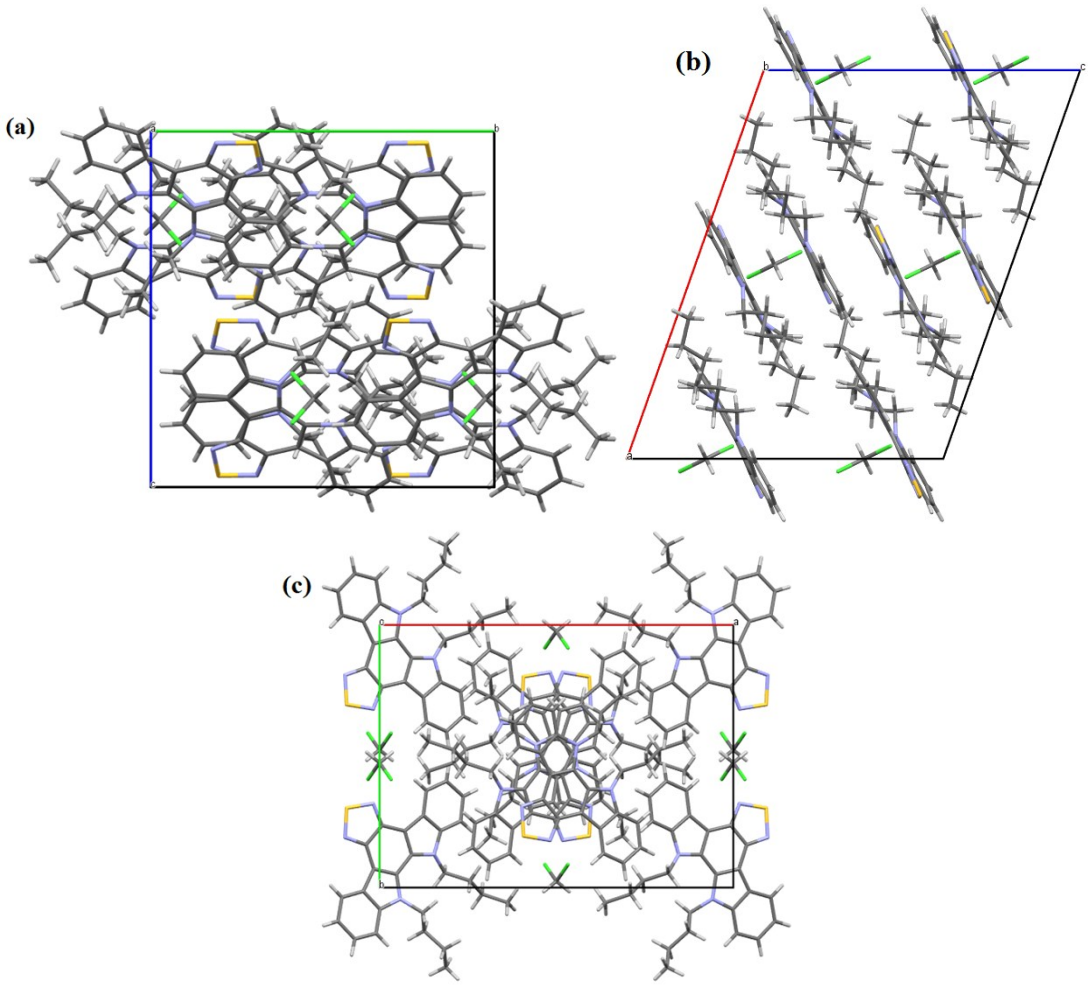


**Figure S2.** Packing diagram of compound **2** along (a) a-axis, (b) b-axis and (c) c-axis.

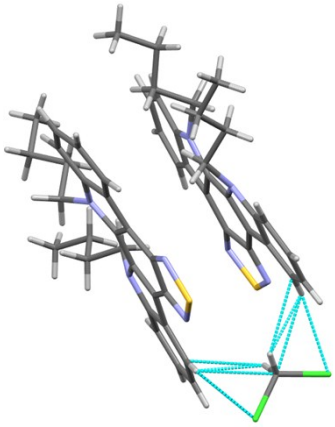

**Figure S3.** Dimerization of compound **2**.

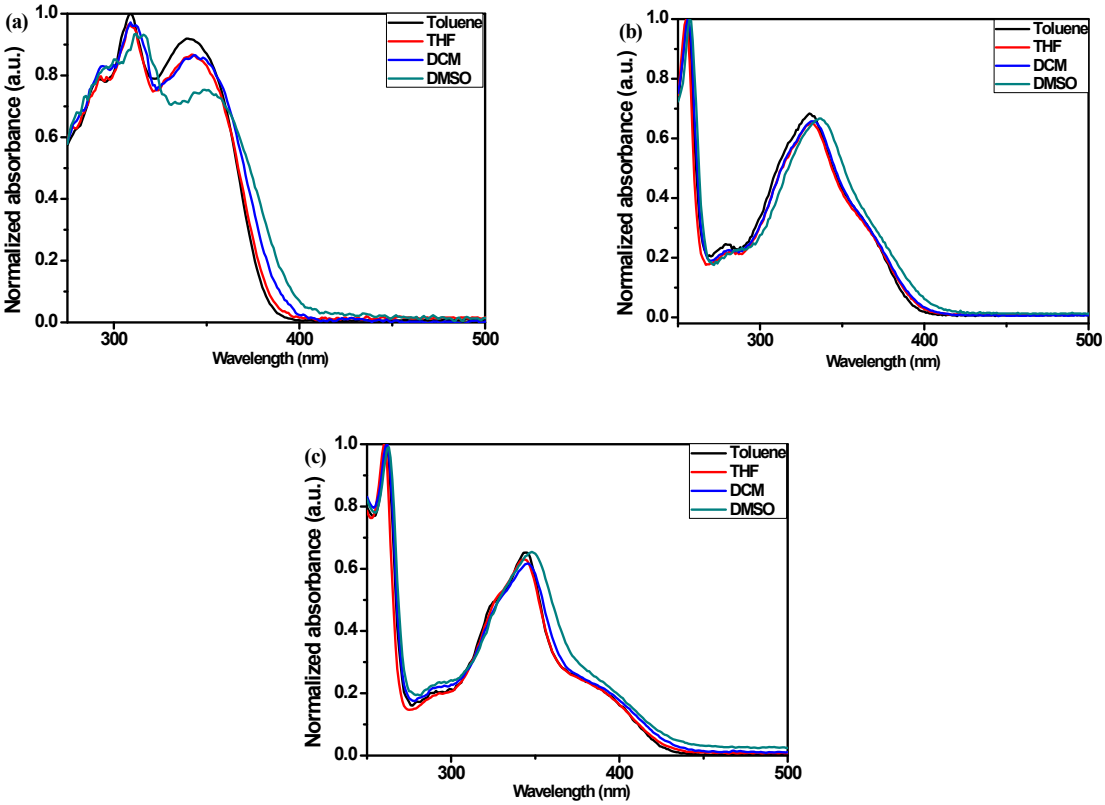


**Figure S4.** Solution state absorption spectra of compounds (a) **1**, (b) **2** and (c) **3**.

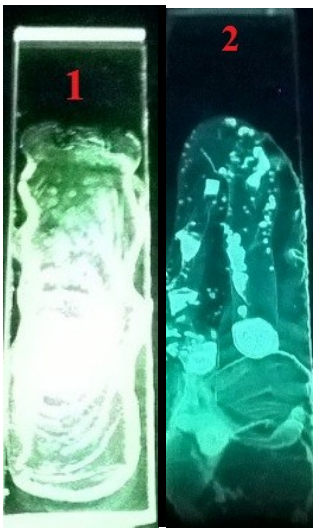


**Figure S5.** Photograph of **1** and **2** in solid state as thin film under 365 nm UV-lamp.

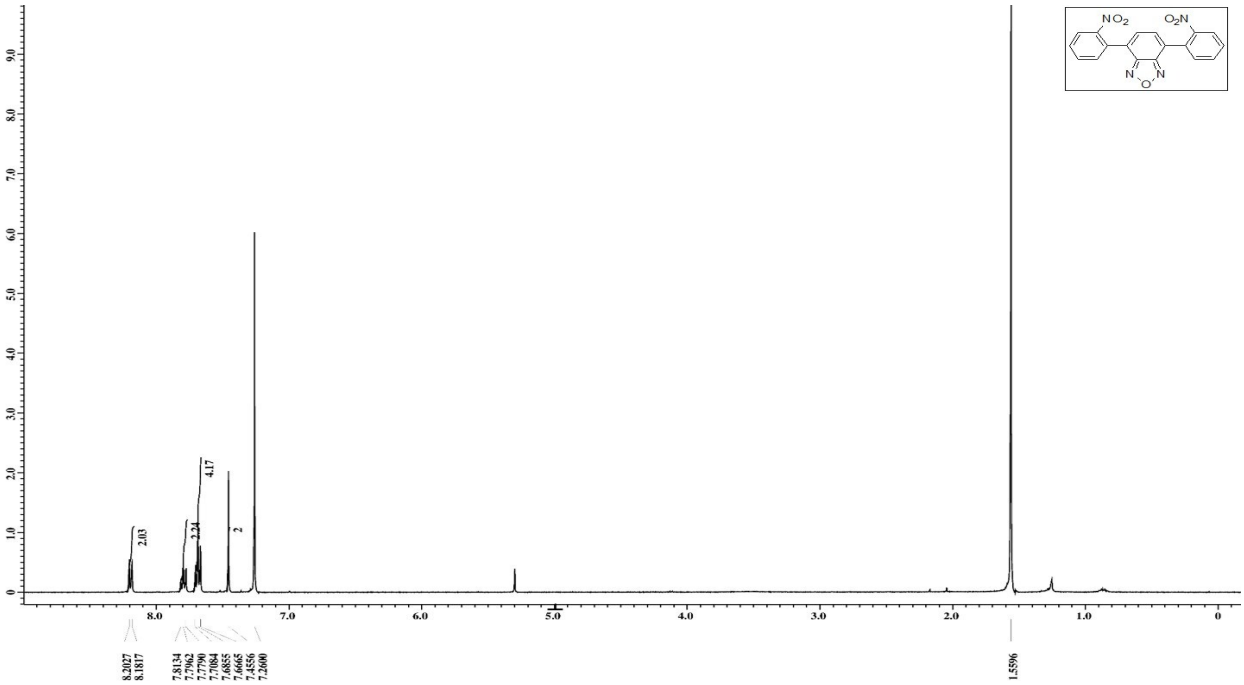


**Figure S6.** $^{1}$H NMR of compound **6a.**

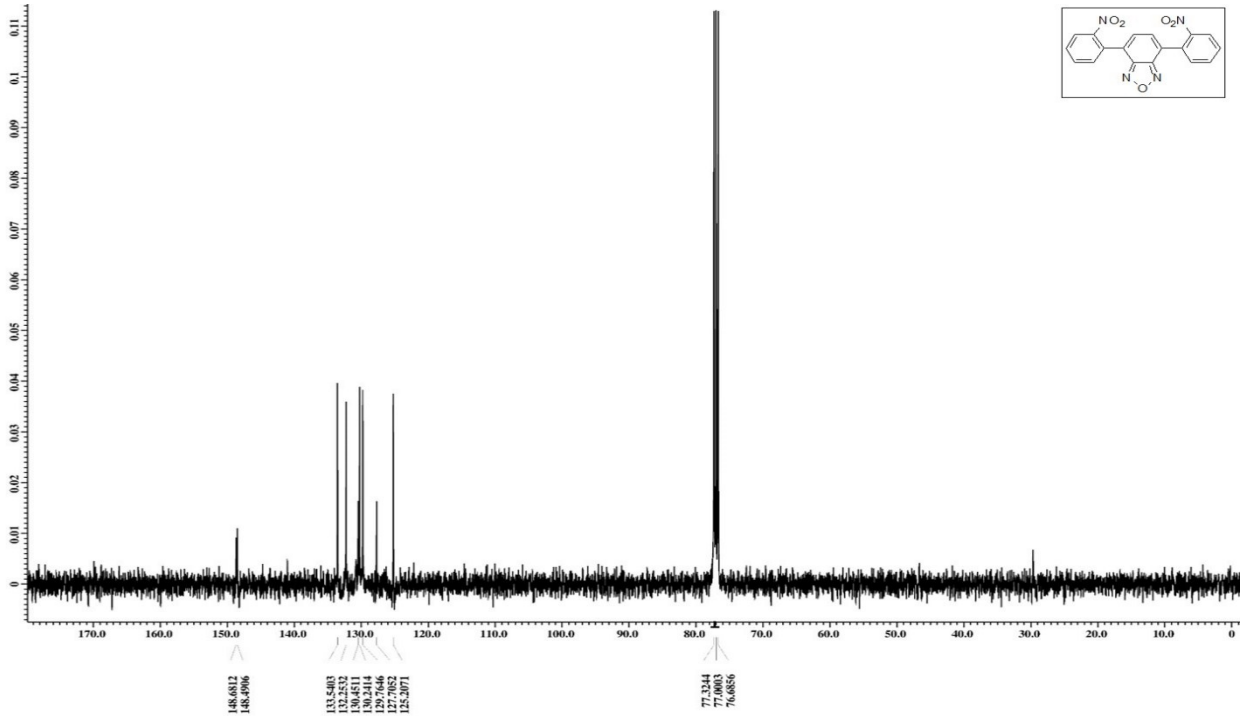


**Figure S7.** $^{13}$C NMR of compound **6a.**

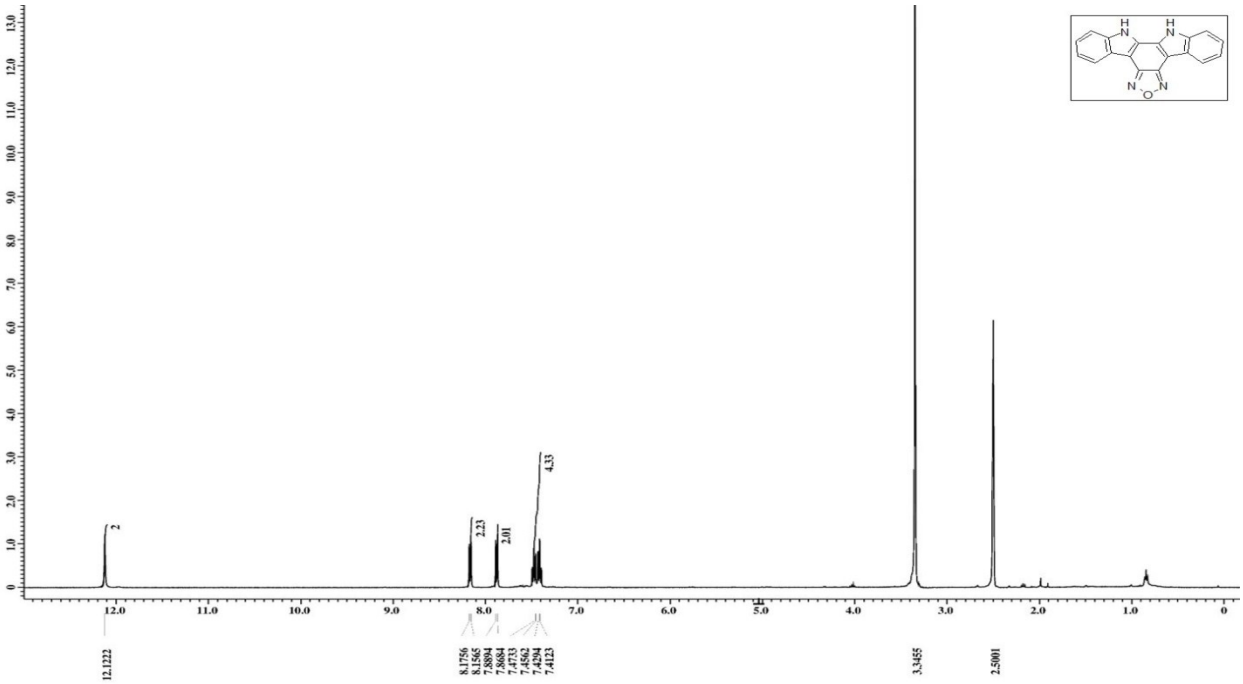


**Figure S8.** $^{1}$H NMR of compound **8a.**

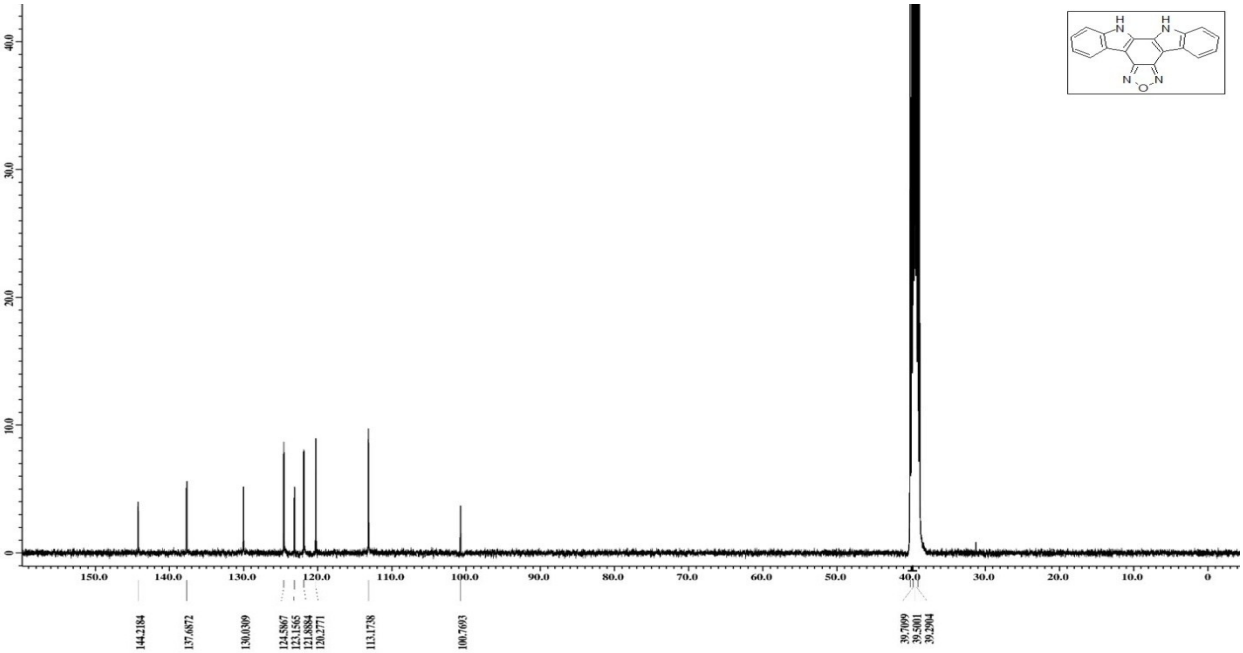


**Figure S9.** $^{13}$C NMR of compound **8a.**

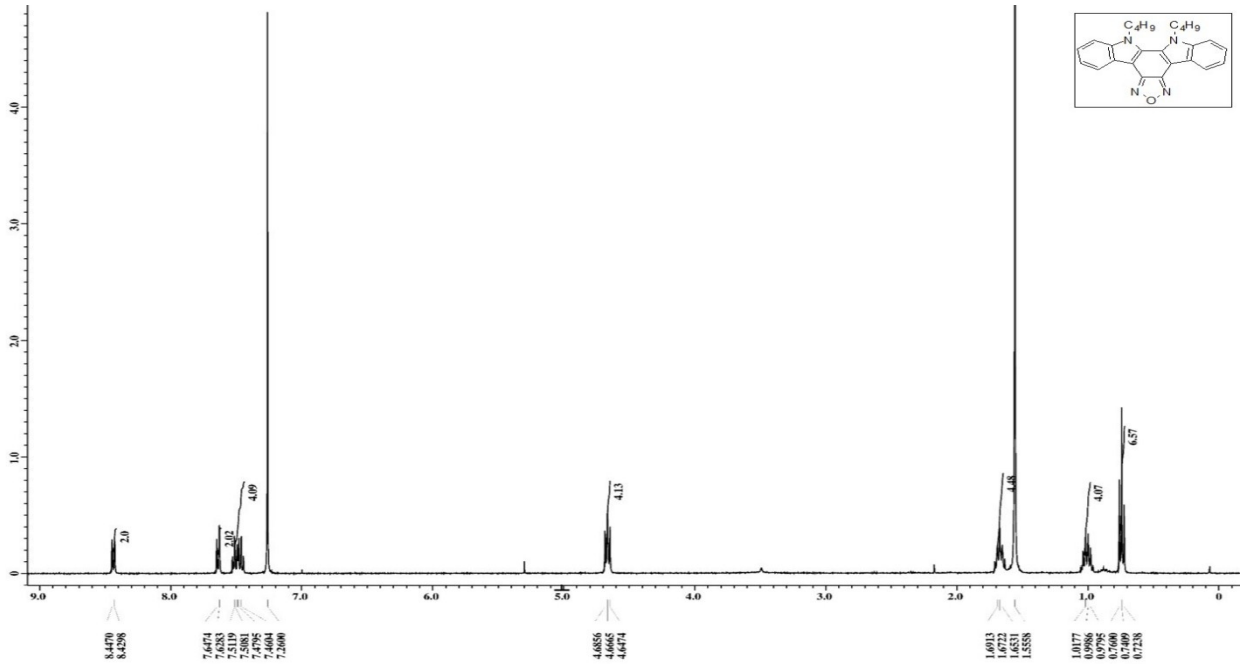

**Figure S10.** $^{1}$H NMR of compound **1.**

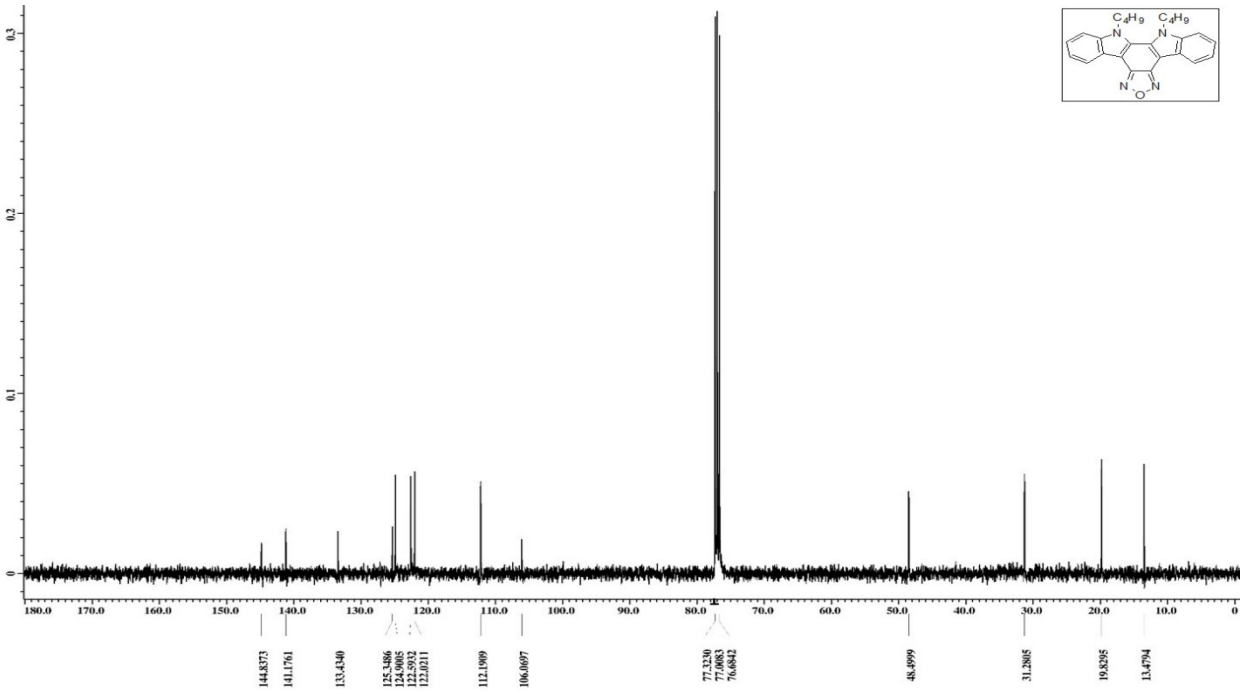

**Figure S11.** $^{13}$C NMR of compound **1.**

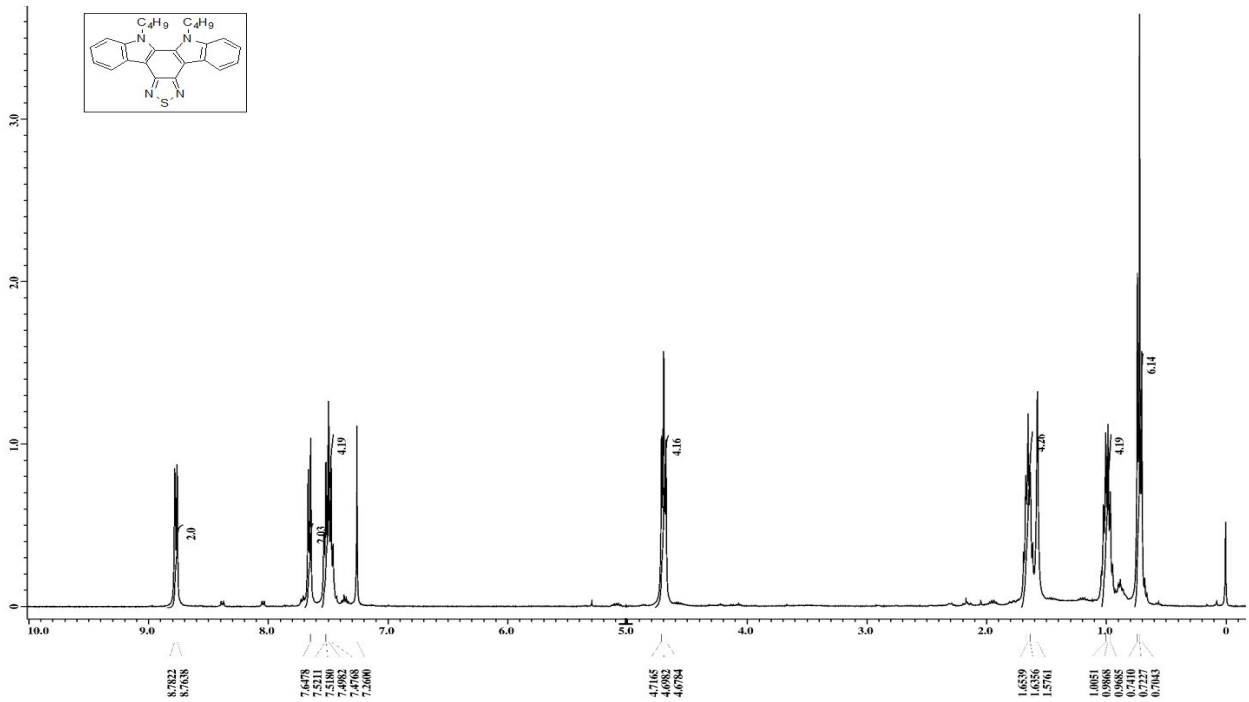

**Figure S12.** $^{1}$H NMR of compound **2.**

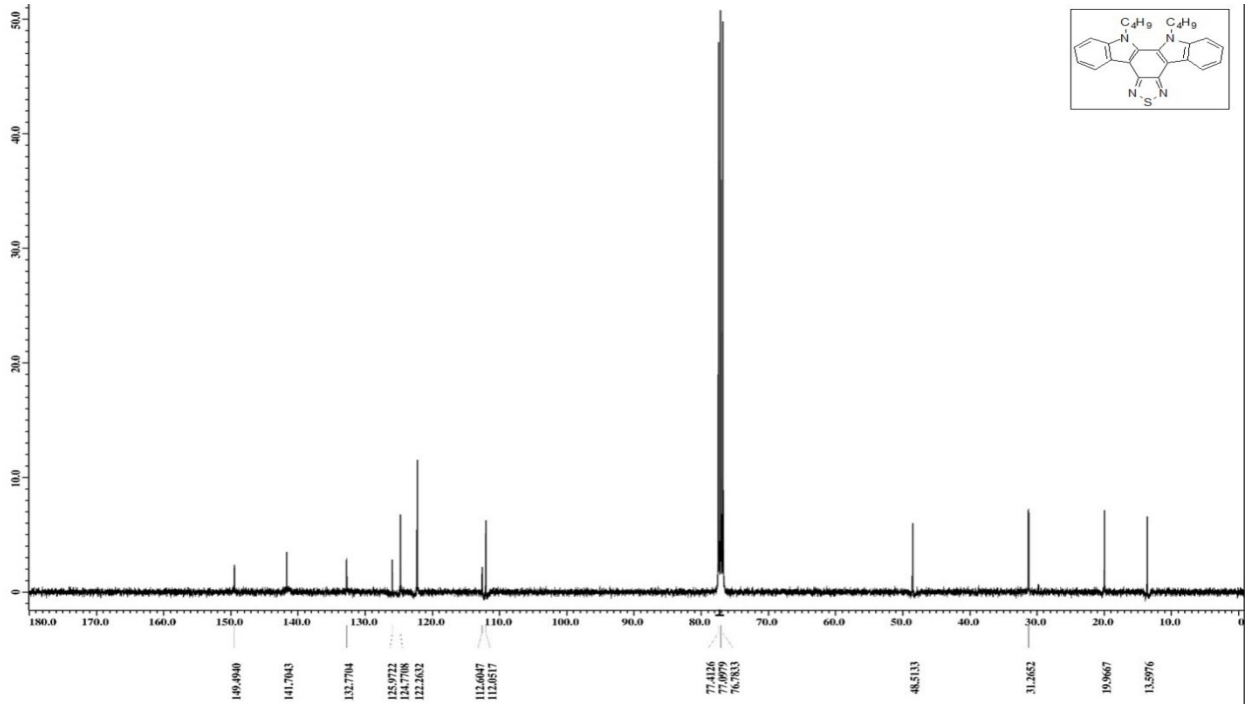

**Figure S13.** $^{13}$C NMR of compound **2.**

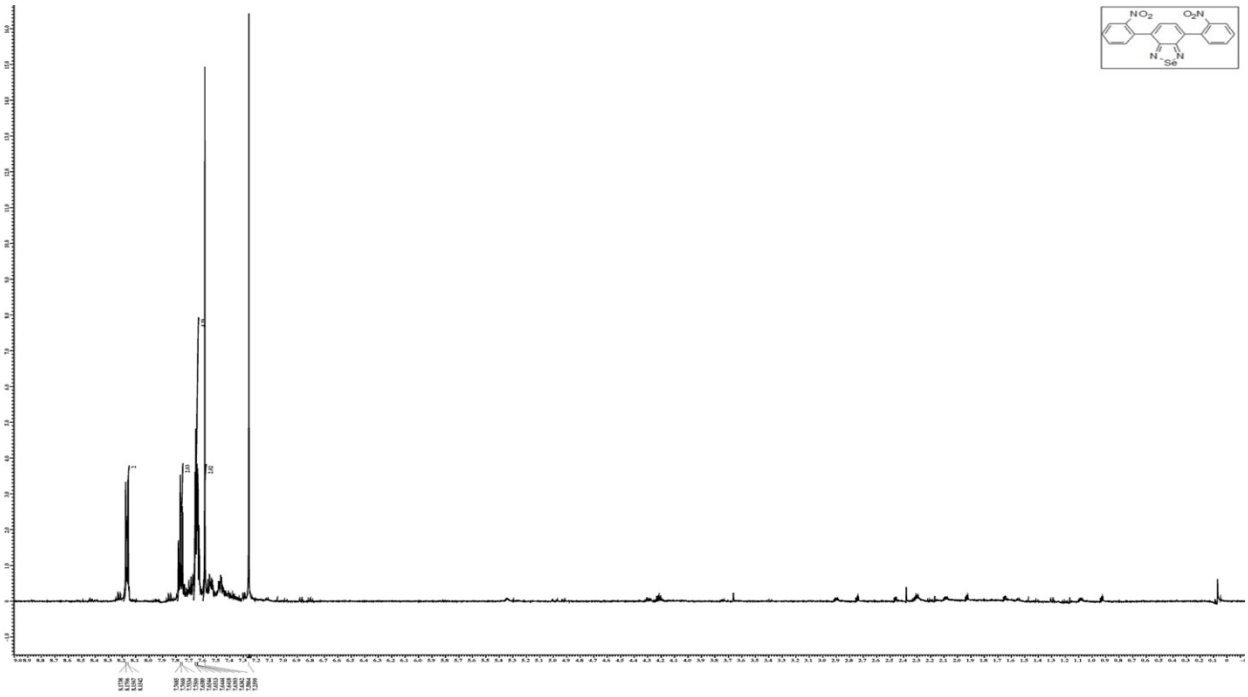

**Figure S14.** $^{1}$H NMR of compound **6b.**

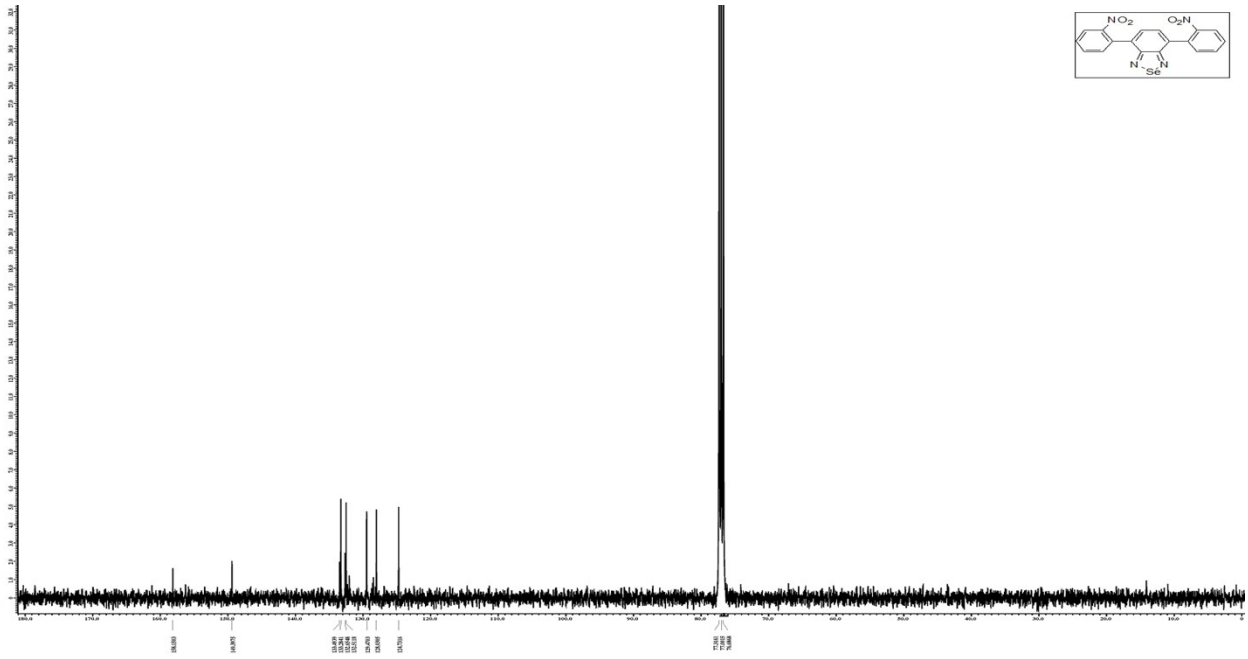

**Figure S15.** $^{13}$C NMR of compound **6b.**

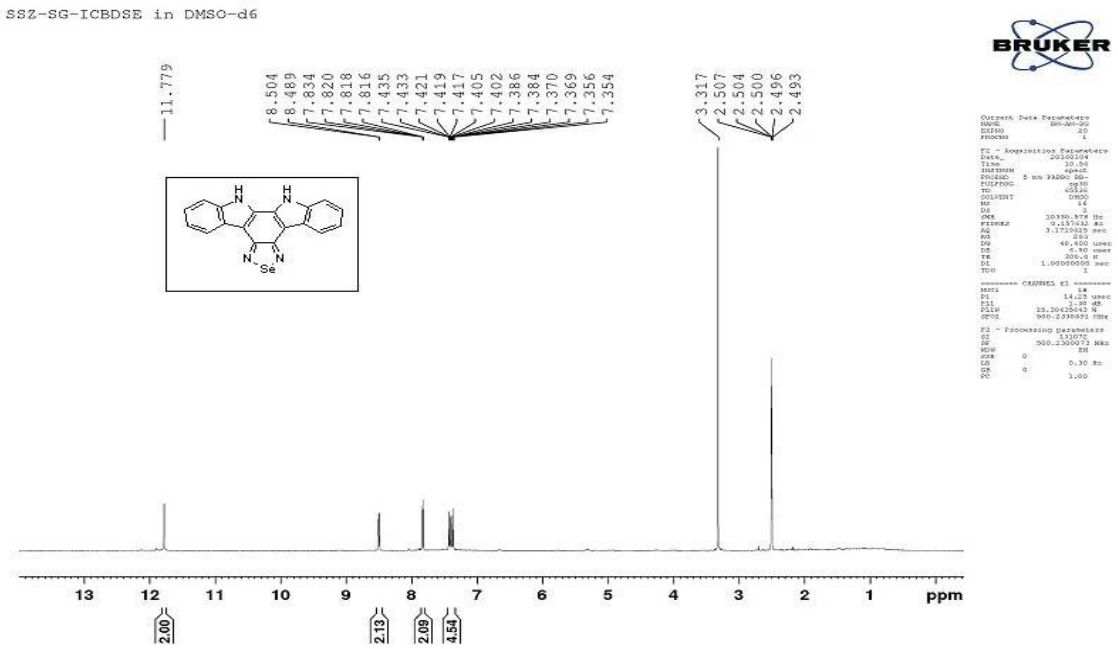


**Figure S16.** $^{1}$H NMR of compound **8c.**

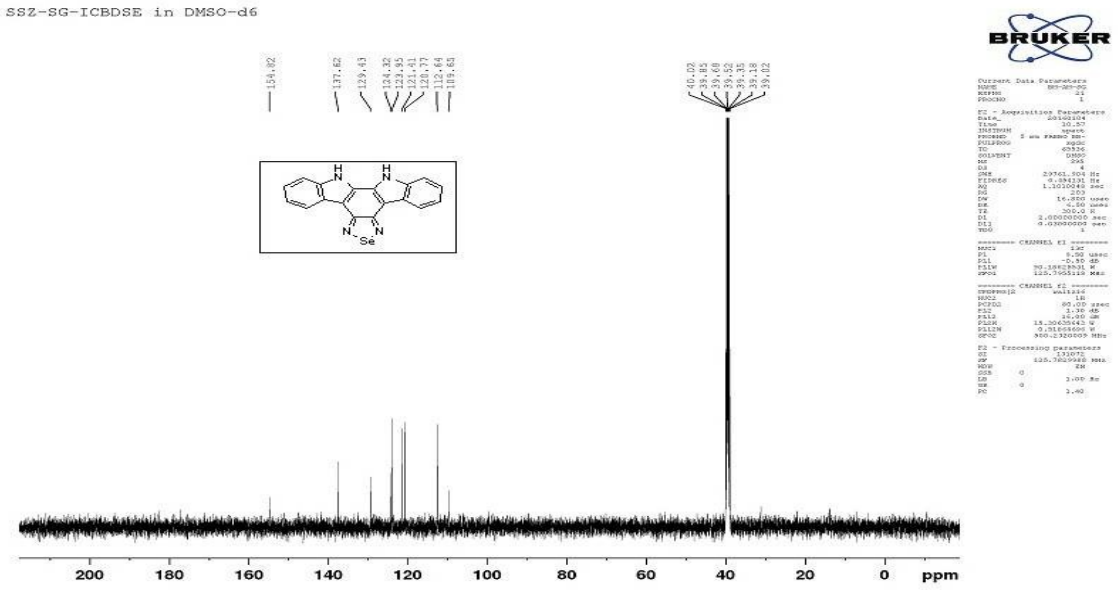


**Figure S17.** $^{13}$C NMR of compound **8c.**

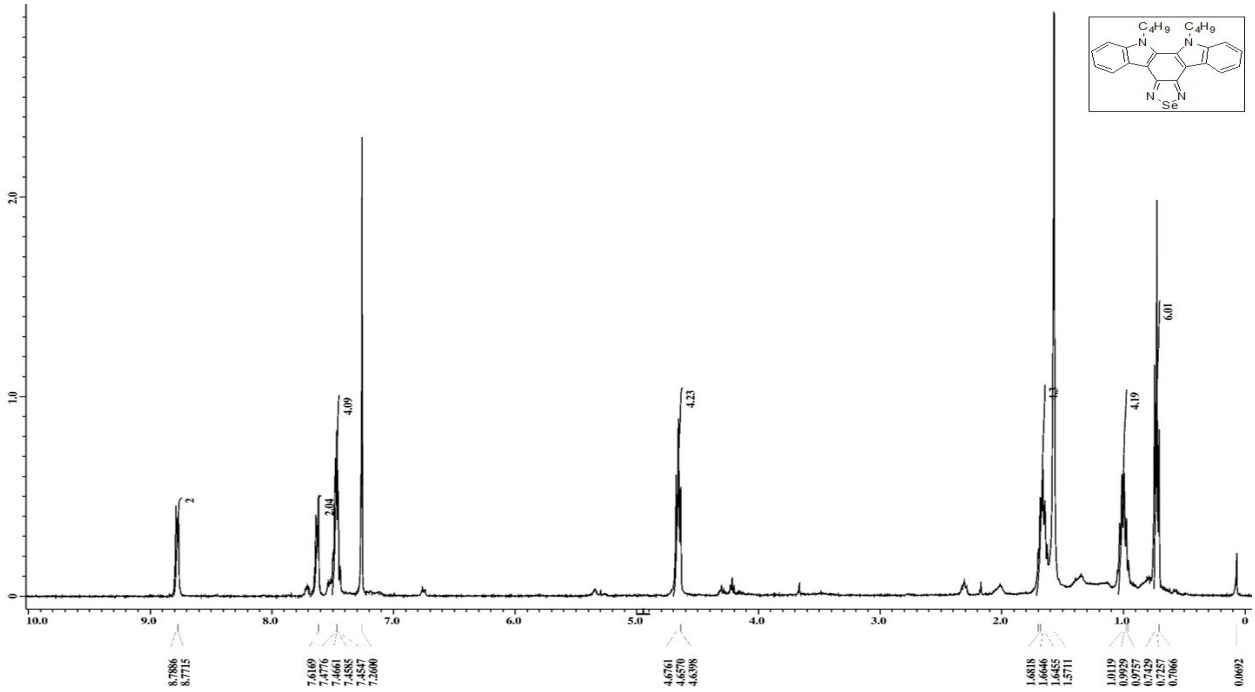

**Figure S18.** $^{1}$H NMR of compound **3.**

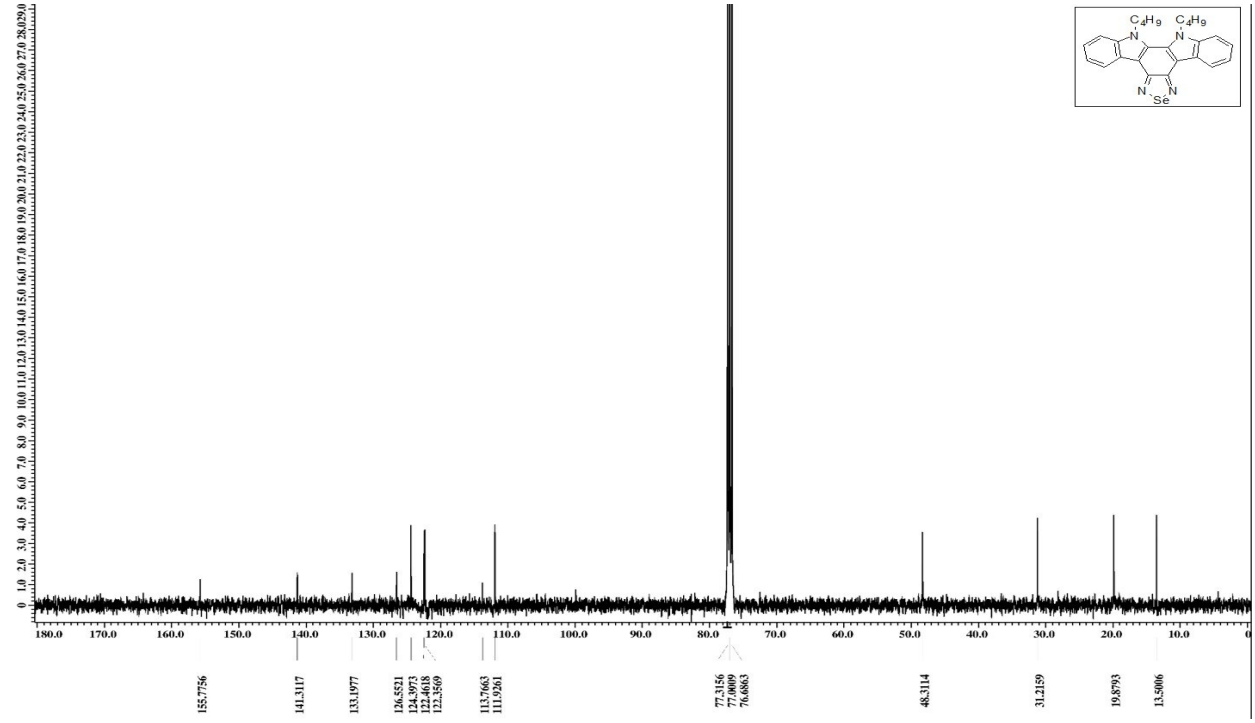

**Figure S19.** $^{13}$C NMR of compound **3.**

**Reference**

T. L. Tam, H. Li, Y. M. Lam, S. G. Mhaisalkar and A. C. Grimsdale, *Org. Lett.*, 2011, **13**, 4613.

**Coordinates for optimized geometry**
**1**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 8 | 0 | 0.007501 | -5.092534 | 0.000088 |
| 2 | 7 | 0 | -1.676193 | 0.401344 | 0.083146 |
| 3 | 7 | 0 | 1.143901 | -4.326362 | 0.140537 |
| 4 | 7 | 0 | 1.675046 | 0.406268 | -0.083121 |
| 5 | 7 | 0 | -1.131141 | -4.329685 | -0.140391 |
| 6 | 6 | 0 | -1.419582 | -1.849824 | -0.118179 |
| 7 | 6 | 0 | -4.209244 | 0.423483 | 0.155167 |
| 8 | 1 | 0 | -4.327632 | 1.490517 | 0.307039 |
| 9 | 6 | 0 | 0.727446 | -0.626720 | 0.003127 |
| 10 | 6 | 0 | -2.821830 | -1.575630 | -0.122056 |
| 11 | 6 | 0 | 4.208032 | 0.435845 | -0.155352 |
| 12 | 1 | 0 | 4.323295 | 1.503213 | -0.307277 |
| 13 | 6 | 0 | -0.725545 | -0.628843 | -0.003037 |
| 14 | 6 | 0 | -1.514126 | 1.731446 | 0.677683 |
| 15 | 1 | 0 | -0.486967 | 1.824821 | 1.028429 |
| 16 | 1 | 0 | -2.148555 | 1.768444 | 1.573690 |
| 17 | 6 | 0 | -1.892516 | 2.895919 | -0.252241 |
| 18 | 1 | 0 | -1.185051 | 2.960249 | -1.088204 |
| 19 | 1 | 0 | -2.868108 | 2.696157 | -0.709009 |
| 20 | 6 | 0 | 1.884061 | 2.901451 | 0.252315 |
| 21 | 1 | 0 | 2.860555 | 2.704795 | 0.708503 |
| 22 | 1 | 0 | 1.176854 | 2.963340 | 1.088718 |
| 23 | 6 | 0 | 3.969147 | -2.378945 | 0.192415 |
| 24 | 1 | 0 | 3.866157 | -3.453323 | 0.308275 |
| 25 | 6 | 0 | 1.425085 | -1.845653 | 0.118263 |
| 26 | 6 | 0 | -2.949566 | -0.175599 | 0.026774 |
| 27 | 6 | 0 | 2.950120 | -0.166918 | -0.026855 |
| 28 | 6 | 0 | 0.715751 | -3.081427 | 0.088485 |
| 29 | 6 | 0 | 1.508953 | 1.735896 | -0.677579 |
| 30 | 1 | 0 | 0.481468 | 1.826258 | -1.028147 |
| 31 | 1 | 0 | 2.143131 | 1.774782 | -1.573675 |
| 32 | 6 | 0 | 5.330805 | -0.384612 | -0.087041 |
| 33 | 1 | 0 | 6.316805 | 0.062923 | -0.176613 |
| 34 | 6 | 0 | -0.706621 | -3.083505 | -0.088363 |
| 35 | 6 | 0 | -1.944307 | 4.238043 | 0.491009 |
| 36 | 1 | 0 | -2.667966 | 4.166448 | 1.315131 |
| 37 | 1 | 0 | -0.971075 | 4.439943 | 0.959895 |
| 38 | 6 | 0 | -2.324479 | 5.409159 | -0.420523 |
| 39 | 1 | 0 | -1.599881 | 5.532305 | -1.234728 |
| 40 | 1 | 0 | -2.361073 | 6.350867 | 0.137793 |
| 41 | 1 | 0 | -3.309490 | 5.252443 | -0.876293 |
| 42 | 6 | 0 | -3.962072 | -2.390599 | -0.192538 |
| 43 | 1 | 0 | -3.855913 | -3.464671 | -0.308378 |
| 44 | 6 | 0 | 2.826517 | -1.567316 | 0.122020 |
| 45 | 6 | 0 | 5.216177 | -1.776072 | 0.093909 |

| | | | | | |
|---|---|---|---|---|---|
| 46 | 1 | 0 | 6.115077 | -2.383611 | 0.146411 |
| 47 | 6 | 0 | -5.329605 | -0.400263 | 0.086799 |
| 48 | 1 | 0 | -6.316923 | 0.044372 | 0.176284 |
| 49 | 6 | 0 | -5.210872 | -1.791381 | -0.094127 |
| 50 | 1 | 0 | -6.107979 | -2.401560 | -0.146687 |
| 51 | 6 | 0 | 1.931020 | 4.243839 | -0.490768 |
| 52 | 1 | 0 | 2.653906 | 4.174538 | -1.315769 |
| 53 | 1 | 0 | 0.956641 | 4.442894 | -0.958473 |
| 54 | 6 | 0 | 2.308853 | 5.415953 | 0.420437 |
| 55 | 1 | 0 | 3.295034 | 5.262226 | 0.874692 |
| 56 | 1 | 0 | 1.585112 | 5.536694 | 1.235770 |
| 57 | 1 | 0 | 2.341667 | 6.357880 | -0.137747 |

Rotational constants (GHZ): 0.1508496 0.1469719 0.0754900

**2**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 16 | 0 | 5.185561 | 0.000114 | 0.000095 |
| 2 | 7 | 0 | -0.605908 | -1.671541 | 0.074401 |
| 3 | 7 | 0 | 4.113644 | -1.254610 | -0.161878 |
| 4 | 7 | 0 | -0.605980 | 1.671502 | -0.074470 |
| 5 | 7 | 0 | 4.113584 | 1.254794 | 0.162030 |
| 6 | 6 | 0 | -1.922656 | -1.506407 | 0.697305 |
| 7 | 6 | 0 | 2.896935 | -0.718583 | -0.092593 |
| 8 | 6 | 0 | 0.428006 | 0.723203 | 0.004580 |
| 9 | 6 | 0 | 0.189734 | 5.326450 | -0.059005 |
| 10 | 6 | 0 | -0.630727 | -4.203877 | 0.134218 |
| 11 | 6 | 0 | 0.428039 | -0.723191 | -0.004565 |
| 12 | 6 | 0 | -1.922745 | 1.506264 | -0.697297 |
| 13 | 6 | 0 | 1.371493 | -2.817731 | -0.134946 |
| 14 | 6 | 0 | 2.896899 | 0.718718 | 0.092689 |
| 15 | 6 | 0 | 1.650626 | 1.413485 | 0.120914 |
| 16 | 6 | 0 | -4.431986 | -1.940963 | 0.568514 |
| 17 | 6 | 0 | -0.028951 | -2.945247 | 0.012429 |
| 18 | 6 | 0 | 1.371352 | 2.817795 | 0.134912 |
| 19 | 6 | 0 | 2.182454 | -3.960066 | -0.213566 |
| 20 | 6 | 0 | 1.650696 | -1.413406 | -0.120872 |
| 21 | 6 | 0 | 0.189984 | -5.326453 | 0.058770 |
| 22 | 6 | 0 | 1.580414 | -5.208863 | -0.122766 |
| 23 | 6 | 0 | 1.580164 | 5.208936 | 0.122595 |
| 24 | 6 | 0 | -0.029092 | 2.945235 | -0.012538 |
| 25 | 6 | 0 | -0.630921 | 4.203834 | -0.134421 |
| 26 | 6 | 0 | 2.182257 | 3.960173 | 0.213495 |
| 27 | 6 | 0 | -3.108827 | -1.878601 | -0.207345 |
| 28 | 6 | 0 | -5.625911 | 2.308777 | 0.318303 |
| 29 | 6 | 0 | -3.108893 | 1.878448 | 0.207394 |
| 30 | 6 | 0 | -5.625854 | -2.308907 | -0.318162 |
| 31 | 6 | 0 | -4.432091 | 1.940737 | -0.568399 |
| 32 | 1 | 0 | 3.255787 | -3.853215 | -0.329077 |
| 33 | 1 | 0 | 2.189056 | -6.106794 | -0.181888 |
| 34 | 1 | 0 | -0.257131 | -6.313249 | 0.142697 |

| | | | | | |
|---|---|---|---|---|---|
| 35 | 1 | 0 | -1.698060 | -4.320333 | 0.285819 |
| 36 | 1 | 0 | 3.255589 | 3.853377 | 0.329065 |
| 37 | 1 | 0 | 2.188760 | 6.106900 | 0.181680 |
| 38 | 1 | 0 | -0.257425 | 6.313221 | -0.143001 |
| 39 | 1 | 0 | -1.698255 | 4.320232 | -0.286073 |
| 40 | 1 | 0 | -1.943848 | -2.141461 | 1.593678 |
| 41 | 1 | 0 | -2.005150 | -0.478614 | 1.050006 |
| 42 | 1 | 0 | -1.944021 | 2.141265 | -1.593710 |
| 43 | 1 | 0 | -2.005199 | 0.478450 | -1.049930 |
| 44 | 1 | 0 | -4.339475 | -2.675693 | 1.380744 |
| 45 | 1 | 0 | -4.621952 | -0.974343 | 1.055868 |
| 46 | 1 | 0 | -3.195811 | -1.162474 | -1.033661 |
| 47 | 1 | 0 | -2.918707 | -2.849094 | -0.678891 |
| 48 | 1 | 0 | -5.480334 | 3.287119 | 0.791879 |
| 49 | 1 | 0 | -6.553316 | 2.354037 | -0.262973 |
| 50 | 1 | 0 | -5.769734 | 1.572653 | 1.118631 |
| 51 | 1 | 0 | -3.195819 | 1.162337 | 1.033731 |
| 52 | 1 | 0 | -2.918771 | 2.848955 | 0.678909 |
| 53 | 1 | 0 | -5.769713 | -1.572700 | -1.118408 |
| 54 | 1 | 0 | -5.480307 | -3.287201 | -0.791846 |
| 55 | 1 | 0 | -6.553229 | -2.354221 | 0.263158 |
| 56 | 1 | 0 | -4.622082 | 0.974064 | -1.055641 |
| 57 | 1 | 0 | -4.339625 | 2.675381 | -1.380712 |

Rotational constants (GHZ): 0.1470032 0.1323058 0.0705609

**3**

| Center Number | Atomic Number | Atomic Type | Coordinates (Angstroms) X | Y | Z |
|---|---|---|---|---|---|
| 1 | 7 | 0 | 1.006983 | 1.671791 | 0.077757 |
| 2 | 7 | 0 | -3.686683 | 1.313466 | -0.174357 |
| 3 | 7 | 0 | 1.006986 | -1.671761 | -0.078029 |
| 4 | 7 | 0 | -3.686646 | -1.313524 | 0.174595 |
| 5 | 6 | 0 | 2.325185 | 1.506627 | 0.697056 |
| 6 | 6 | 0 | -2.505778 | 0.725321 | -0.094447 |
| 7 | 6 | 0 | -0.025822 | -0.723732 | 0.004190 |
| 8 | 6 | 0 | 0.207046 | -5.325633 | -0.063349 |
| 9 | 6 | 0 | 1.029285 | 4.204282 | 0.138934 |
| 10 | 6 | 0 | -0.025836 | 0.723746 | -0.004264 |
| 11 | 6 | 0 | 2.325259 | -1.506517 | -0.697127 |
| 12 | 6 | 0 | -0.970761 | 2.814605 | -0.133972 |
| 13 | 6 | 0 | -2.505757 | -0.725361 | 0.094574 |
| 14 | 6 | 0 | -1.248109 | -1.409823 | 0.121339 |
| 15 | 6 | 0 | 4.834174 | 1.941062 | 0.562168 |
| 16 | 6 | 0 | 0.429184 | 2.945078 | 0.015668 |
| 17 | 6 | 0 | -0.970701 | -2.814619 | 0.133836 |
| 18 | 6 | 0 | -1.783279 | 3.955930 | -0.213010 |
| 19 | 6 | 0 | -1.248143 | 1.409803 | -0.121327 |
| 20 | 6 | 0 | 0.206948 | 5.325658 | 0.062870 |
| 21 | 6 | 0 | -1.183070 | 5.205480 | -0.120697 |
| 22 | 6 | 0 | -1.182962 | -5.205499 | 0.120347 |
| 23 | 6 | 0 | 0.429229 | -2.945055 | -0.015978 |
| 24 | 6 | 0 | 1.029353 | -4.204237 | -0.139387 |

| | | | | | |
|---|---|---|---|---|---|
| 25 | 6 | 0 | -1.783187 | -3.955971 | 0.212838 |
| 26 | 6 | 0 | 3.508841 | 1.880723 | -0.210118 |
| 27 | 6 | 0 | 6.025473 | -2.311266 | 0.327394 |
| 28 | 6 | 0 | 3.508786 | -1.880664 | 0.210204 |
| 29 | 6 | 0 | 6.025576 | 2.311195 | -0.326921 |
| 30 | 6 | 0 | 4.834247 | -1.940953 | -0.561858 |
| 31 | 1 | 0 | -2.855714 | 3.844898 | -0.329856 |
| 32 | 1 | 0 | -1.793102 | 6.102515 | -0.180179 |
| 33 | 1 | 0 | 0.652262 | 6.313187 | 0.147908 |
| 34 | 1 | 0 | 2.096276 | 4.322064 | 0.292260 |
| 35 | 1 | 0 | -2.855611 | -3.844970 | 0.329810 |
| 36 | 1 | 0 | -1.792970 | -6.102552 | 0.179779 |
| 37 | 1 | 0 | 0.652374 | -6.313148 | -0.148490 |
| 38 | 1 | 0 | 2.096339 | -4.321975 | -0.292796 |
| 39 | 1 | 0 | 2.348084 | 2.140792 | 1.593984 |
| 40 | 1 | 0 | 2.409191 | 0.478520 | 1.048442 |
| 41 | 1 | 0 | 2.348297 | -2.140639 | -1.594085 |
| 42 | 1 | 0 | 2.409285 | -0.478395 | -1.048444 |
| 43 | 1 | 0 | 4.744003 | 2.673765 | 1.376482 |
| 44 | 1 | 0 | 5.025439 | 0.973182 | 1.046516 |
| 45 | 1 | 0 | 3.593351 | 1.166452 | -1.038320 |
| 46 | 1 | 0 | 3.317392 | 2.852345 | -0.678780 |
| 47 | 1 | 0 | 5.878526 | -3.290842 | 0.797985 |
| 48 | 1 | 0 | 6.954597 | -2.354970 | -0.251262 |
| 49 | 1 | 0 | 6.166892 | -1.577235 | 1.130074 |
| 50 | 1 | 0 | 3.593157 | -1.166442 | 1.038464 |
| 51 | 1 | 0 | 3.317249 | -2.852312 | 0.678773 |
| 52 | 1 | 0 | 6.167135 | 1.577023 | -1.129448 |
| 53 | 1 | 0 | 5.878737 | 3.290692 | -0.797710 |
| 54 | 1 | 0 | 6.954590 | 2.354982 | 0.251903 |
| 55 | 1 | 0 | 5.025645 | -0.973010 | -1.046025 |
| 56 | 1 | 0 | 4.744193 | -2.673533 | -1.376297 |
| 57 | 34 | 0 | -4.919740 | -0.000037 | 0.000170 |

Rotational constants (GHZ): 0.1468920 0.1009672 0.0605232