# Electronic Supplementary Information

## DFT study of electron donor-acceptor (EDA) complexes: mechanism exploration and theoretical prediction

Zhao Liu,‡[a,b] Shutao Wang,‡ [a,b] Zhiqiang Liu,‡ [a,b] Yating Ding,[a] Yansong Hu,[b] Runzhang Liu,[b] Zhengze Zhang,[b] Yi-Feng Qiu*[c] and Junqiang Lei *[a]

[a] First Hospital of Lanzhou University, Lanzhou University, 222 South Tianshui Road, Lanzhou 730000 (P. R. China).

[b] State Key Laboratory of Applied Organic Chemistry, College of Chemistry and Chemical Engineering, Lanzhou University.

[c] College of Chemistry and Chemical Engineering, Northwest Normal University, 967 East Anning Road, Lanzhou 730070 (P. R. China).

*E-mail: leijq2011@126.com and qyfnet@nwnu.edu.cn

# Contents

## 1. Computation details

All calculations were carried out with the Gaussian 09 programs.[1] The geometries of all the species were fully optimized by using density functional theory (DFT) of the 6-2X method [2] with the 6-311 G (d, p) basis set for all atoms. Frequency analysis was used to determine the minimum point of the optimized conformation and obtain its energy at the same level of theory. Finally, it should note that this method has been widely applied successfully in a variety of chemical conversion process of theoretical research.[3] The convergence criteria are used as default and the vibrational analysis has also been carried out at standard conditions (1 atm, 298.15 K). The solvent effects are represented by the implicit solvent model using the SMD-$CH_3OH$ model.[4] Analysis of interaction region indicator (IRI) was performed with the Multiwfn program.[5] The 3D structure of molecules is drawn by CYL-View[6] and VMD.[7] The obtained molecular structure is directly used for single point time-dependent density functional (TD-DFT) calculation at the level of CAM-B3LYP /6-311++G (d, p).

## 2. The substituted benzyl bromide molecules selected

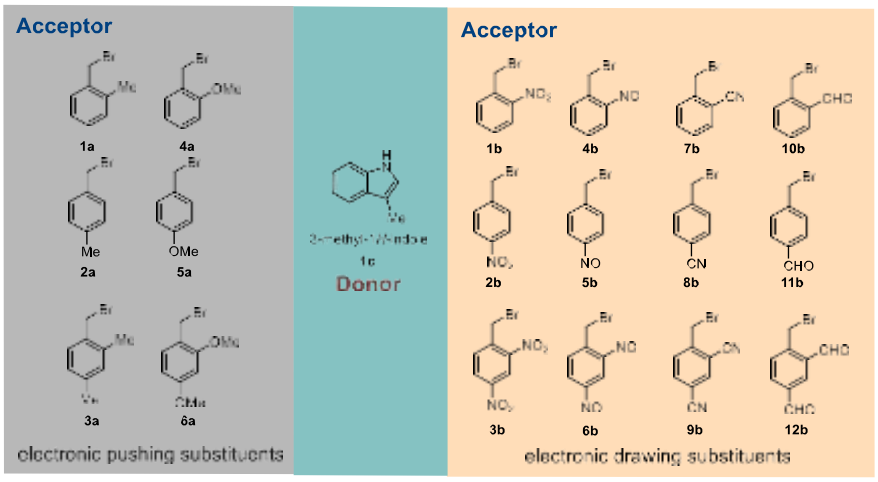



**Fig. S1** The substituted benzyl bromide molecules selected in this study.

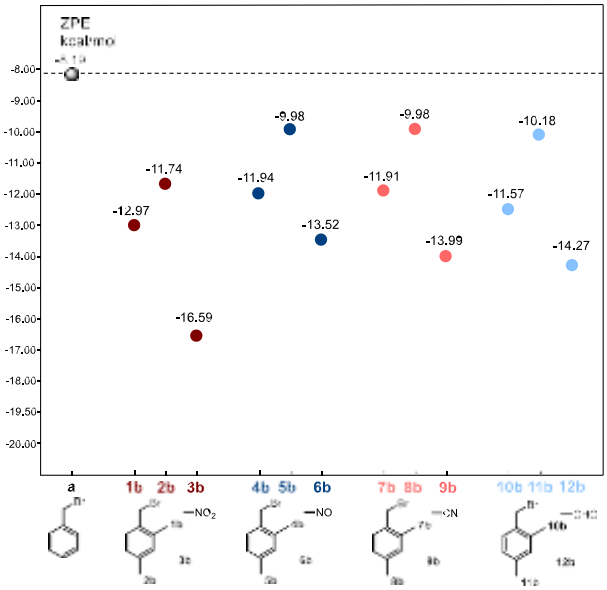



**Fig. S2** The formation energy of the selected EDA complex (electron-withdrawing group).

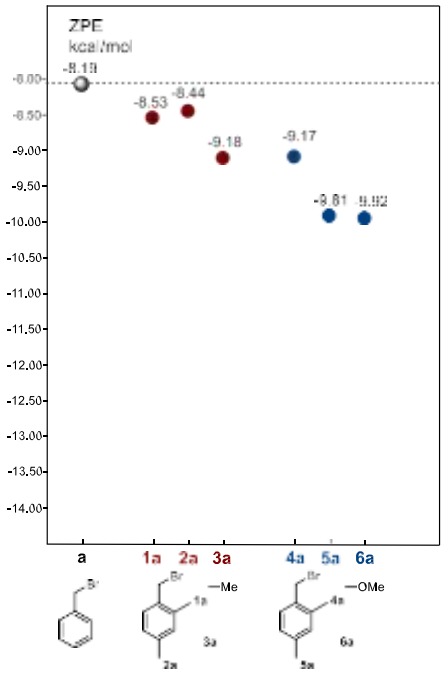



**Fig. S3** The formation energy of the selected EDA complex (electron-donating group).

## 3. The substituted 1H-indoles molecules selected

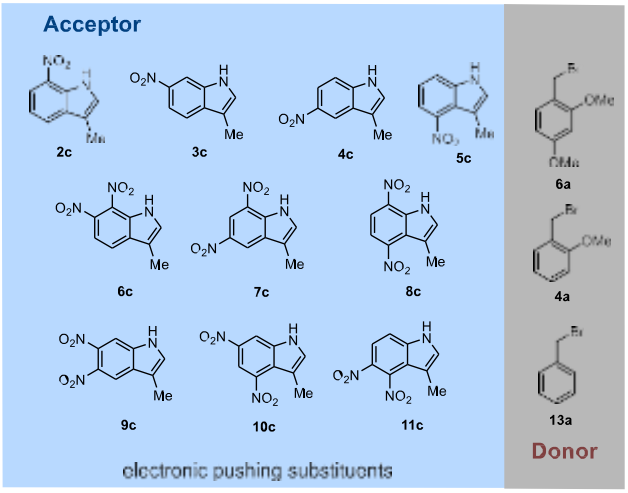



**Fig. S4** The substituted 1H-indoles molecules selected in this study.

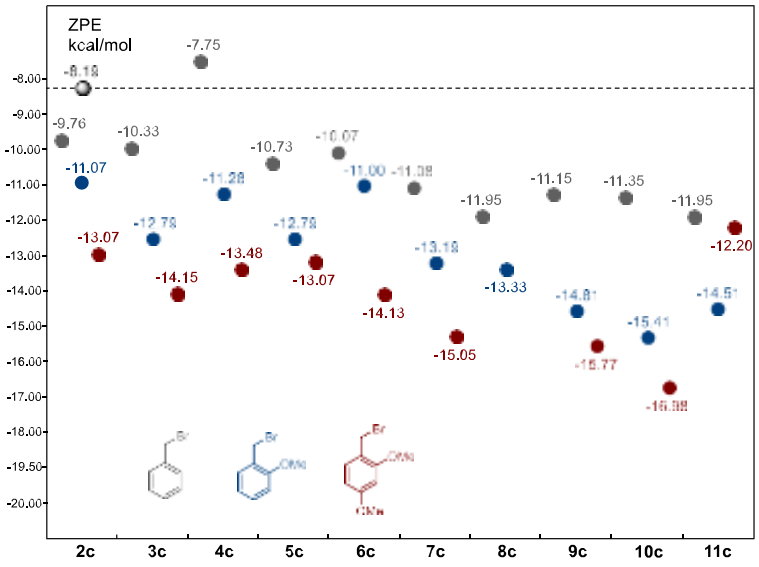



**Fig. S5** The formation energy of the selected EDA complex (electron-withdrawing group).

## 4. The other mothed, evaluate dispersion effects and basis set superposition error (BSSE) for calculating the binding energy

**Table S1** The other mothed for calculating the binding energy. [a]

| EDA Complexes | M062X/6-311G** | B3LYP/6-311G** | M06L/6-311G** | M062X/6-31G | M062X/6-31G** |
|---|---|---|---|---|---|
| **3b-1c** | -14.70 | -113.35 | -13.19 | -14.09 | -13.46 |
| **13a-1c** | -6.92 | 58.64 | -6.26 | -6.34 | -6.21 |
| **6a-1c** | -9.90 | -111.13 | -9.08 | -8.85 | -9.20 |
| **3b-10c** | -15.73 | -3.13 | -14.16 | -14.83 | -14.74 |
| **13a-10c** | -10.57 | -1.24 | -9.61 | -9.75 | -9.51 |
| **6a-10c** | -15.22 | -2.74 | -13.95 | -13.96 | -13.72 |
| **3b-methylpyrrole** | -9.61 | -1.16 | -9.14 | -9.90 | -9.50 |

[a] All units are in kcal /mol and without BSSE correction.

Besides M06-2X/6-311-G**, we also tried the B3LYP and M06-L functional, 6-31G and 6-31G** basis set (in without dispersion effect correction and BSSE correction of, as shown in table S1). We found that the B3LYP functional does not provide a proper description of the binding of the EDA complex (the binding energy was grossly overestimated). Relative to M06-2X, although M06-L can also be the result of the binding energy gives a reasonable, but M06-2X more common in the field of organic system[8] and M06-L is often used in the system containing metal.[9]

**Table S2** The basis set superposition error (BSSE) for the binding energy. [a]

| EDA Complexes | Before correction | Value of correction | After correction |
|---|---|---|---|
| **3b-1c** | -14.70 | 4.40 | -10.30 |
| **13a-1c** | -6.92 | 1.66 | -5.26 |
| **6a-1c** | -9.90 | 2.66 | -7.24 |
| **3b-10c** | -15.73 | 5.53 | -10.2 |
| **13a-10c** | -10.57 | 3.19 | -7.38 |
| **6a-10c** | -15.22 | 5.13 | -10.09 |
| **3b-methylpyrrole** | -9.61 | 3.07 | -6.54 |

[a] All units are in kcal /mol.

**Table S3** The evaluate dispersion effects for the binding energy. [a]

| EDA Complexes | Before correction | DFT-D3(0) correction | Percentage error |
|---|---|---|---|
| **3b-1c** | -14.70 | -16.06 | -9.25% |
| **13a-1c** | -6.92 | -6.38 | 7.83% |
| **6a-1c** | -9.90 | -11.38 | -15.04% |
| **3b-10c** | -15.73 | -17.45 | -10.94% |
| **13a-10c** | -10.57 | -11.91 | -12.70% |
| **6a-10c** | -15.22 | -17.02 | -11.84% |
| **3b-methylpyrrole** | -9.61 | -10.57 | -10.00% |

[a] All units are in kcal /mol.

As shown in table 3, D3 (0) correction for M06-2 x's influence on the calculation of the binding energy of EDA complex is acceptable, the maximum is 15%. It is because of M06-2X is more accurate for attractive noncovalent interactions.

## 5. Distance measurement of two molecules in EDA complexes

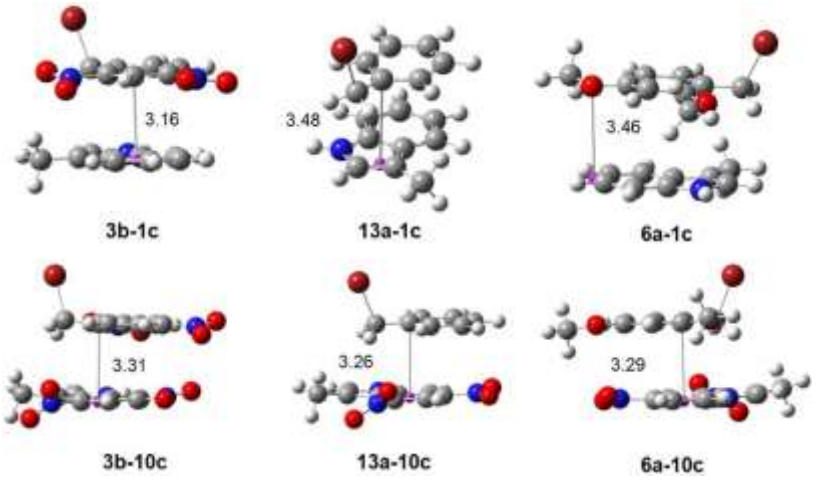



**Fig. S6** The distance of two molecules in EDA complexes.

## 6. The FMO analyses of selected substrates

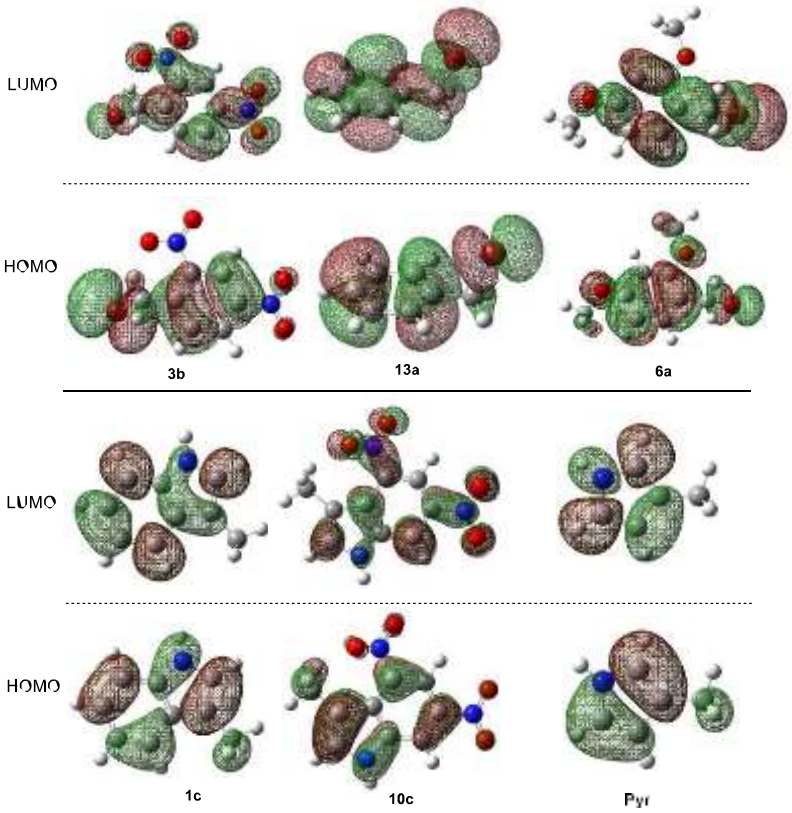



**Fig. S7** The FMO analyses of substrates.

**Table S4** The $E_{HOMO}$, $E_{LUMO}$ and $E_g$ of selected substrates.

| Selected substrates | $E_{HOMO}$/eV | $E_{LUMO}$/eV | $E_g$/eV |
|---|---|---|---|
| **3b** | -9.13 | -2.08 | -7.06 |
| **13a** | -8.23 | -0.14 | -8.10 |
| **6a** | -7.36 | 0.06 | -7.42 |
| **1c** | -6.87 | 0.44 | -7.31 |
| **10c** | -7.60 | -1.80 | -5.80 |
| **Pyr** | -7.14 | 2.21 | -9.35 |

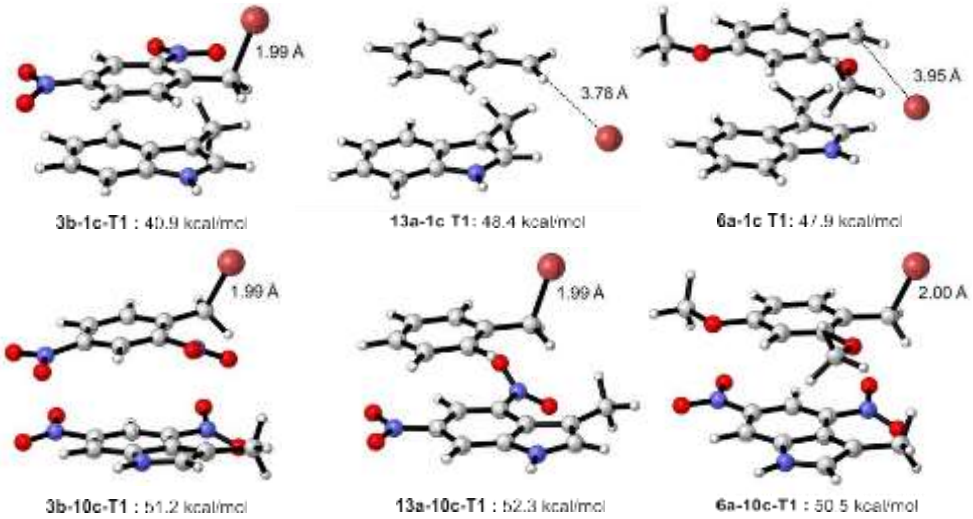


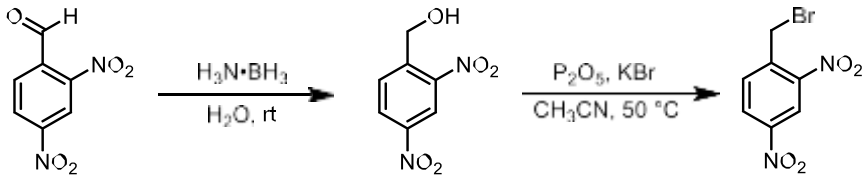

**Fig. S8** Structure of EDA complex in excited triplet state.

## 7. General information and synthesis of compound 3b

### 7.1 General information

Unless otherwise noted, all reagents were purchased from commercial sources and used as received without further purification. Benzyl bromide, 3-methylpyrrole, 3-methylindole, and 2, 4-dinitrobenzaldehyde were purchased from Bide Pharmaceutical. Unless otherwise indicated, all experiments were carried out under air atmosphere. The silica gel (200-300 meshes) was used for column chromatography and TLC inspections were taken on silica gel GF254 plates. Liquid $^{1}H$ and $^{13}C$ NMR spectra were recorded on a Bruker Avance III 400 MHz spectrometer.

### 7.2 Synthesis of compound 3b

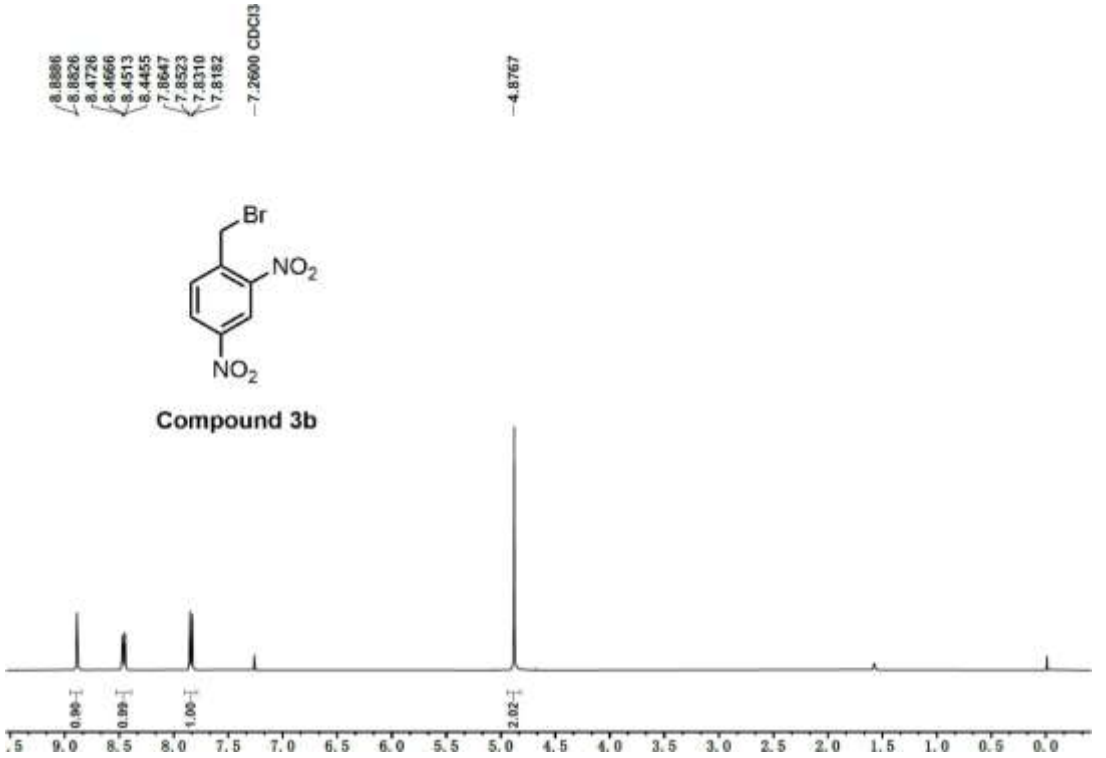


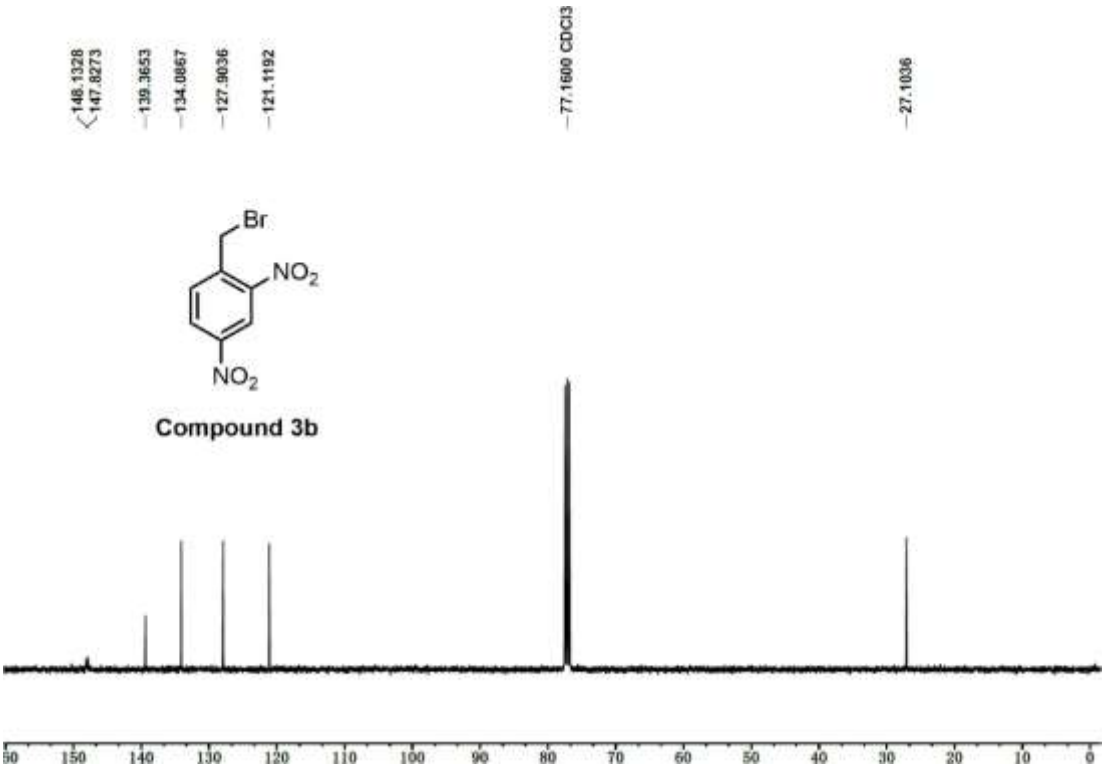

Compound 3b

2,4-dinitrobenzaldehyde (5 mmol) and ammonia-borane (5 mmol) were dissolved in 20 mL $H_2O$, the resulting solution was then stirred at room temperature. After completion of the reaction as monitored by TLC, the reaction mixture was extracted with EA. The combined organic layers were then washed with brine, dried over $Na_2SO_4$, the solvent was removed under vacuo, the crude product was obtained and proceeded directly to the next step without any purification.

(2,4-dinitrophenyl)methanol (2 mmol), potassium bromide (3 mmol) and phosphorus pentoxide (4 mmol) were added to a 100 mL double-necked round-bottom flask with a magneton and a spherical condensing tube. After replacing the air atmosphere in the system three times with argon, inject 15 ml of dry acetonitrile into it. The resulting solution was then stirred at 50 ℃. After completion of the reaction as monitored by TLC, the mixture was allowed to cool to room temperature before being extracted with EA. The combined organic layers were then washed with brine, dried over $Na_2SO_4$ and filtered. Concentration of the solution under reduced pressure gave the crude product. Purification of the crude product by silica gel column

chromatography (16:1 to 4:1 PE/EA), The $^{1}H$ and $^{13}C$ NMR data of the product were consistent with those reported in the literature.[10] $^{1}H$ NMR (400 MHz, $CDCl_3$) δ = 8.9 (d, *J*=2.4, 1H), 8.5 (dd, *J*=2.4, 8.5, 1H), 7.8 (d, *J*=8.5, 1H), 4.9 (s, 2H). $^{13}C$ NMR (101 MHz, $CDCl_3$) δ = 148.1, 147.8, 139.4, 134.1, 127.9, 121.1, 27.1.



**Experimental UV-Vis spectra of 3b-methylpyrrole**

The UV/Vis absorption spectra were recorded in 1 cm path quartz cuvettes by using a Varian Cary 300 Conc UV/Vis spectrometer, respectively. Sample preparation method: **3b** (0.125 mmol) and **3-methylpyrrole** (0.125 mmol) was dissolved in 10 mL MeOH. The same amount of **3b** and **3-methylpyrrole** of the substance was dissolved in 20 ml of methanol and stirred for 10min before testing.

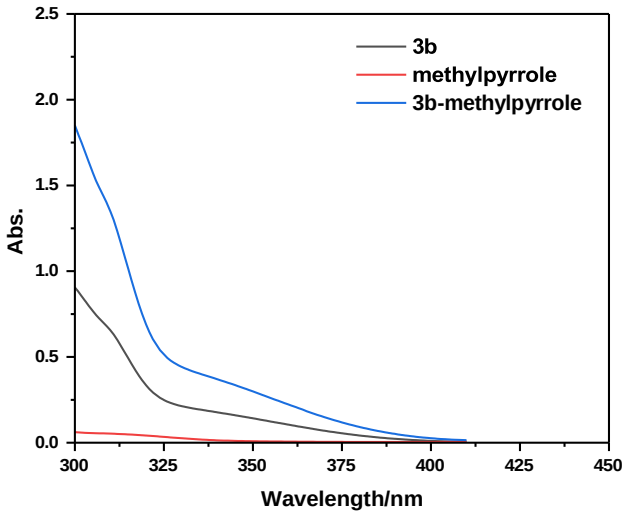



**Fig. S9** UV-Vis spectra of 3b, 3-methylpyrrole and 3b-methylpyrrole.

## 8. References


1. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision D.01, Gaussian, Inc., Wallingford, CT, 2013.
2. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, 120, 215-241.
3. a) R. Fang, L. Zhou, P.-C. Tu, A. M. Kirillov and L. Yang, *Organometallics*, 2018, 37, 1927-1936. b) M. Citroni, F. Datchi, R. Bini, M. Di Vaira, P. Pruzan, B. Canny and V. Schettino, *J. Phys. Chem. B*, 2008, 112, 1095-1103. c) Y. Zhao and D. G. Truhlar, *J. Chem. Theory. Comput.*, 2008, 4, 1849-1868. d) Y. Zhao and D. G. Truhlar, *Acc Chem. Res.*, 2008, 41, 157-167. e) D. Jacquemin, E. A. Perpete, I. Ciofini, C. Adamo, R. Valero, Y. Zhao and D. G. Truhlar, *J. Chem. Theory Comput.*, 2010, 6, 2071-2085. f) P.-C. Tu, L. Zhou, A. M. Kirillov, R. Fang and L. Yang, *Org. Chem. Front.*, 2018, 5, 1356-1365.
4. A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, 113, 6378-6396.
5. T. Lu and F. Chen, *J. Comput. Chem.*, 2012, 33, 580-592.
6. C. Y. Legault, Cylview, 1.0 b, Universit´e de Sherbrooke, Sherbrooke, Canada, 2009.
7. Humphrey W, Dalke A, Schulten K, *J. Molec. Graphics.*, 1996, 14, 33-38.
8. a) T. Bai and J. Ling, *J. Phys. Chem. A*, 2017, 121, 4588-4593. b) P. C. Tu, L. Zhou,

A. M. Kirillov, R. Fang and L. Z. Yang, *Org. Chem. Front.*, 2018, 5, 1356-1365. c) L. Zhou, L. Yang, S. S. Dai, Y. Y. Gao, R. Fang, A. M. Kirillov and L. Z. Yang, *Catal. Sci. Technol.*, 2020, 10, 240-251.

9. a) D. J. Xiao, E. D. Bloch, J. A. Mason, W. L. Queen, M. R. Hudson, N. Planas, J. Borycz, A. L. Dzubak, P. Verma, K. Lee, F. Bonino, V. Crocella, J. Yano, S. Bordiga, D. G. Truhlar, L. Gagliardi, C. M. Brown and J. R. Long, *Nat. Chem.*, 2014, 6, 590-595. b) P. Verma, K. D. Vogiatzis, N. Planas, J. Borycz, D. J. Xiao, J. R. Long, L. Gagliardi and D. G. Truhlar, *J. Am. Chem. Soc.*, 2015, 137, 5770-5781. c) S. Ketrat, T. Maihom, S. Wannakao, M. Probst, S. Nokbin and J. Limtrakul, *Inorg. Chem.*, 2017, 56, 14005-14012.
10. E. B. McLean, V. Gauchot, S. Brunen, D. J. Burns and A. L. Lee, *Chem. Commun.*, 2019, 55, 4238-4241.

## 9. Cartesian coordinates

**3b-1c**

0 1

| | | | |
|---|---|---|---|
| Br | 3.93393600 | -0.97535900 | -0.07349900 |
| N | -2.62722900 | -2.42166700 | 0.54847600 |
| O | -3.16866700 | -3.07567500 | -0.31734300 |
| O | -3.12038500 | -2.18223000 | 1.62947200 |
| C | 2.39658100 | -0.02951400 | -0.86419200 |
| H | 2.51046300 | 1.00815800 | -0.58006500 |
| H | 2.50018300 | -0.15298000 | -1.93878900 |
| C | 1.11651600 | -0.65207300 | -0.39756100 |
| C | 0.54573700 | -1.62815700 | -1.22301700 |
| H | 1.05818100 | -1.89814600 | -2.13902200 |
| C | -0.65962700 | -2.23435100 | -0.91980700 |
| H | -1.10093800 | -2.96709000 | -1.58201500 |
| C | -1.30203300 | -1.86402500 | 0.25249800 |
| C | -0.78249700 | -0.92916400 | 1.11985900 |
| H | -1.30415200 | -0.64799200 | 2.02270300 |
| C | 0.42065100 | -0.32969200 | 0.77489400 |
| N | -0.52113700 | 1.44338300 | -2.24801400 |
| H | -0.33106400 | 1.02152200 | -3.14567000 |
| C | 0.28183100 | 2.36306400 | -1.61508000 |
| H | 1.19288900 | 2.70628100 | -2.08395600 |
| C | -0.26394400 | 2.72463800 | -0.41062600 |
| C | -1.48913800 | 1.97610300 | -0.29204600 |

| | | | |
|---|---|---|---|
| C | -2.46978200 | 1.87109400 | 0.70797300 |
| H | -2.38955300 | 2.45551500 | 1.61892300 |
| C | -3.53114400 | 1.00220100 | 0.51554700 |
| H | -4.29205700 | 0.90417300 | 1.28166100 |
| C | -3.64730000 | 0.24206900 | -0.66662200 |
| H | -4.49239800 | -0.42767300 | -0.78576800 |
| C | -2.69427500 | 0.31935200 | -1.66772700 |
| H | -2.77146300 | -0.27522800 | -2.57147500 |
| C | -1.61391000 | 1.18413700 | -1.46181600 |
| C | 0.27983400 | 3.73034700 | 0.55621200 |
| H | 0.38815600 | 3.31481900 | 1.56244000 |
| H | -0.38413600 | 4.59615900 | 0.63846600 |
| H | 1.25867100 | 4.08625100 | 0.22878800 |
| N | 0.88960900 | 0.71175400 | 1.70197900 |
| O | 0.10972700 | 1.10770200 | 2.54444100 |
| O | 2.02379500 | 1.12561700 | 1.59070900 |

**13a-1c**

0 1

| | | | |
|---|---|---|---|
| Br | -3.88378200 | 0.03037300 | 0.27711500 |
| C | -1.99288300 | 0.63231600 | 0.13549700 |
| H | -1.99351600 | 1.35259400 | -0.67892900 |
| H | -1.79003600 | 1.12550200 | 1.08223100 |
| C | -1.07740100 | -0.51796100 | -0.11714600 |
| C | -0.45189000 | -1.16562900 | 0.94720200 |

| | | | |
|---|---|---|---|
| H | -0.64615300 | -0.83581400 | 1.96329600 |
| C | 0.42605600 | -2.21983800 | 0.70968400 |
| H | 0.91545300 | -2.71250200 | 1.54228700 |
| C | 0.68119900 | -2.63358000 | -0.59406000 |
| C | 0.05502800 | -1.99169100 | -1.66202700 |
| H | 0.25482100 | -2.30882400 | -2.67935700 |
| C | -0.82137700 | -0.94027500 | -1.42390700 |
| N | 1.36998900 | 1.73293600 | 1.50581400 |
| H | 1.16800700 | 1.92754400 | 2.47559400 |
| C | 0.79920600 | 2.37520100 | 0.42788100 |
| H | 0.05825500 | 3.14644600 | 0.58141500 |
| C | 1.31163700 | 1.88529100 | -0.74202600 |
| C | 2.26415700 | 0.87362700 | -0.36648100 |
| C | 3.09933800 | 0.01227400 | -1.09608800 |
| H | 3.10347700 | 0.04066400 | -2.18128400 |
| C | 3.90875300 | -0.87588900 | -0.40900700 |
| H | 4.55756000 | -1.54946000 | -0.95748300 |
| C | 3.90374000 | -0.92150300 | 1.00024400 |
| H | 4.54935500 | -1.62815800 | 1.50965800 |
| C | 3.09304000 | -0.08359000 | 1.74695000 |
| H | 3.08632700 | -0.11964100 | 2.83068900 |
| C | 2.27432900 | 0.80988400 | 1.04929100 |
| C | 0.94109500 | 2.28000700 | -2.13601000 |
| H | 0.55573600 | 1.42308600 | -2.69771900 |
| H | 1.80489900 | 2.66477800 | -2.68656100 |

| | | | |
|---|---|---|---|
| H | 0.17243100 | 3.05553900 | -2.13001100 |
| H | -1.30989300 | -0.43869000 | -2.25369000 |
| H | 1.37155800 | -3.44853800 | -0.77986800 |

**6a-1c**

0 1

| | | | |
|---|---|---|---|
| Br | 4.01296500 | 0.38686300 | 0.07632700 |
| C | 2.31631700 | -0.26556400 | -0.75771200 |
| H | 2.52467900 | -0.25982800 | -1.82365300 |
| H | 2.21780800 | -1.28138600 | -0.38644700 |
| C | 1.15917500 | 0.59487100 | -0.41169800 |
| C | 0.49252500 | 0.43471000 | 0.82083800 |
| C | -0.60138100 | 1.22554400 | 1.13801300 |
| H | -1.14133800 | 1.11606300 | 2.06912900 |
| C | -1.06664800 | 2.16701600 | 0.21292700 |
| C | -0.42134600 | 2.34931800 | -1.00755600 |
| H | -0.76800300 | 3.07355700 | -1.73123500 |
| C | 0.68769000 | 1.55479500 | -1.29485800 |
| N | -1.08162900 | -2.88042600 | 0.76855300 |
| H | -0.98999800 | -3.34676500 | 1.65921500 |
| C | -0.22056400 | -3.02483700 | -0.29814400 |
| H | 0.60912800 | -3.71458000 | -0.23948100 |
| C | -0.59985200 | -2.20805500 | -1.32807300 |
| C | -1.76392200 | -1.49821300 | -0.86523400 |
| C | -2.58412200 | -0.50970800 | -1.43221100 |
| H | -2.39782600 | -0.15335900 | -2.44068000 |

| | | | |
|---|---|---|---|
| C | -3.62361300 | 0.01106500 | -0.67972200 |
| H | -4.26279900 | 0.77944500 | -1.10051100 |
| C | -3.86684600 | -0.44062100 | 0.63331700 |
| H | -4.68667500 | -0.01094200 | 1.19797700 |
| C | -3.08177000 | -1.42154700 | 1.21593600 |
| H | -3.26805100 | -1.77043600 | 2.22574100 |
| C | -2.02840400 | -1.93987300 | 0.45509500 |
| C | 0.06175400 | -2.05097500 | -2.66023100 |
| H | 0.32839800 | -1.00542300 | -2.84583900 |
| H | -0.59810700 | -2.36573300 | -3.47463100 |
| H | 0.97355100 | -2.64951500 | -2.71524000 |
| H | 1.19678500 | 1.68287200 | -2.24513400 |
| O | 0.97937000 | -0.53230400 | 1.63243500 |
| C | 0.37325000 | -0.69967000 | 2.90847300 |
| H | 0.89744400 | -1.52841200 | 3.38029000 |
| H | 0.49407800 | 0.20323300 | 3.51356100 |
| H | -0.68809400 | -0.94212700 | 2.81433300 |
| O | -2.17926800 | 2.84440300 | 0.59616200 |
| C | -2.73860100 | 3.76850000 | -0.32993500 |
| H | -3.63045100 | 4.16719500 | 0.14905100 |
| H | -2.04070200 | 4.58353200 | -0.53970200 |
| H | -3.01484900 | 3.26807100 | -1.26218600 |

**3b-10c**

0 1

| | | | |
|---|---|---|---|
| Br | 2.29708300 | 3.15744500 | -0.39330800 |
| C | 1.58498600 | 1.35372100 | -0.72532100 |
| H | 1.76562200 | 1.15787500 | -1.77885000 |
| H | 2.16695900 | 0.68751800 | -0.09975800 |
| C | 0.11220000 | 1.32131700 | -0.44530400 |
| C | -0.49174500 | 1.15861900 | 0.81107400 |
| C | -1.86782100 | 1.12535300 | 0.97749700 |
| H | -2.30658000 | 0.98241500 | 1.95515900 |
| C | -2.65500300 | 1.23251600 | -0.14994600 |
| C | -2.12153200 | 1.38302100 | -1.42083900 |
| H | -2.76828300 | 1.44741800 | -2.28590000 |
| C | -0.74350500 | 1.43920700 | -1.54719000 |
| N | 1.16448700 | -2.08945800 | 2.51340400 |
| H | 0.75614900 | -2.09221300 | 3.43949500 |
| C | 2.49040100 | -1.97832000 | 2.23116900 |
| H | 3.21764300 | -1.92951900 | 3.02861000 |
| C | 2.70899700 | -1.92144600 | 0.87050100 |
| C | 1.41152500 | -1.99550900 | 0.27722800 |
| C | 0.85994200 | -1.91408400 | -1.01825800 |
| C | -0.49446300 | -1.87336900 | -1.24832300 |
| C | -1.35533800 | -1.94762800 | -0.14990900 |
| C | -0.91229800 | -2.06422800 | 1.15721000 |
| C | 0.46085400 | -2.08158600 | 1.34289000 |
| C | 4.05466700 | -1.72834000 | 0.24123800 |
| H | 4.04283100 | -0.90406100 | -0.47581200 |

| | | | |
|---|---|---|---|
| H | 4.39067800 | -2.62119200 | -0.28883700 |
| H | 4.78477000 | -1.49327100 | 1.01753800 |
| H | -0.30800400 | 1.55547800 | -2.53278100 |
| H | -1.60295900 | -2.09919100 | 1.99064700 |
| N | 1.72255300 | -1.85652100 | -2.19615200 |
| O | 2.74547800 | -2.50670000 | -2.17831000 |
| O | 1.36154100 | -1.17410800 | -3.13580700 |
| H | -0.88285300 | -1.78000500 | -2.25309100 |
| N | -2.78594100 | -1.80549800 | -0.39518500 |
| O | -3.17482500 | -1.78021300 | -1.54536800 |
| O | -3.52299900 | -1.67312600 | 0.56528000 |
| N | -4.11249900 | 1.11304000 | 0.00966200 |
| O | -4.57368500 | 1.23085000 | 1.12337000 |
| O | -4.76625500 | 0.88712300 | -0.98481600 |
| N | 0.29586000 | 0.93845800 | 2.03991600 |
| O | -0.30094000 | 0.59044600 | 3.03811900 |
| O | 1.49465000 | 1.10354700 | 1.99572400 |

**13a-10c**

0 1

| | | | |
|---|---|---|---|
| Br | 3.53755100 | -1.57901000 | -0.20414100 |
| C | 1.84709200 | -0.55721700 | 0.00704200 |
| H | 1.92140600 | -0.11461200 | 0.99781100 |
| H | 1.89039100 | 0.20951900 | -0.76288400 |
| C | 0.65569800 | -1.44555300 | -0.13394400 |

| | | | |
|---|---|---|---|
| C | 0.05332600 | -1.62582400 | -1.37889100 |
| C | -1.07536100 | -2.43126400 | -1.50291800 |
| H | -1.54570800 | -2.55751500 | -2.47171800 |
| C | -1.60822800 | -3.06171500 | -0.38197500 |
| C | -1.01017300 | -2.88432500 | 0.86480900 |
| H | -1.43040900 | -3.36440100 | 1.74126200 |
| C | 0.11839400 | -2.08243400 | 0.98738300 |
| N | -0.73344300 | 2.30247000 | -2.46622800 |
| H | -1.13782500 | 2.21803800 | -3.38947800 |
| C | 0.39500800 | 2.99564600 | -2.15432300 |
| H | 0.93940500 | 3.52930400 | -2.91976300 |
| C | 0.69339500 | 2.88564900 | -0.81303800 |
| C | -0.33722000 | 2.06072600 | -0.26319200 |
| C | -0.64540300 | 1.48231600 | 0.98548700 |
| C | -1.67961500 | 0.59324500 | 1.15788700 |
| C | -2.47379700 | 0.28039600 | 0.05243400 |
| C | -2.27098600 | 0.82044800 | -1.20548500 |
| C | -1.20604800 | 1.69591100 | -1.33744800 |
| C | 1.91496200 | 3.47220900 | -0.17361000 |
| H | 2.45995200 | 2.72204300 | 0.40432100 |
| H | 1.67029100 | 4.29372000 | 0.50183300 |
| H | 2.58097800 | 3.85218900 | -0.95033300 |
| H | 0.58030400 | -1.93465400 | 1.95888400 |
| H | 0.46391100 | -1.12412100 | -2.25038600 |
| H | -2.49661100 | -3.67676700 | -0.47505000 |

| | | | |
|---|---|---|---|
| H | -2.89487100 | 0.54688200 | -2.04648200 |
| N | 0.13708600 | 1.80843600 | 2.17305300 |
| O | 0.55682500 | 2.94149700 | 2.28089500 |
| O | 0.31405900 | 0.93467400 | 3.00092500 |
| H | -1.87337700 | 0.14947100 | 2.12434300 |
| N | -3.53683000 | -0.70154900 | 0.22482100 |
| O | -3.74927400 | -1.13184900 | 1.34132600 |
| O | -4.15112000 | -1.06163500 | -0.76068200 |

**6a-10c**

0 1

| | | | |
|---|---|---|---|
| Br | 2.44556400 | 3.01273700 | -0.49590200 |
| C | 1.54880300 | 1.23516600 | -0.65888100 |
| H | 1.74948500 | 0.92584200 | -1.68151200 |
| H | 2.08374400 | 0.61181400 | 0.05130300 |
| C | 0.09428500 | 1.32453000 | -0.37750200 |
| C | -0.38071100 | 1.28513500 | 0.94911100 |
| C | -1.74005400 | 1.38000800 | 1.21355000 |
| H | -2.13661200 | 1.35186800 | 2.21964400 |
| C | -2.64853900 | 1.47708300 | 0.15308500 |
| C | -2.20444500 | 1.48628900 | -1.16744900 |
| H | -2.89453000 | 1.54416600 | -1.99778000 |
| C | -0.83231700 | 1.42124600 | -1.40560900 |
| N | 0.86370300 | -2.02562800 | 2.59445400 |
| H | 0.43491600 | -1.99989300 | 3.51029000 |

| | | | |
|---|---|---|---|
| C | 2.20010100 | -1.99251900 | 2.34493600 |
| H | 2.90965600 | -1.97437800 | 3.15958800 |
| C | 2.45462600 | -1.97905600 | 0.98983700 |
| C | 1.16949200 | -1.99764700 | 0.36383600 |
| C | 0.65598700 | -1.93283600 | -0.94853800 |
| C | -0.68778100 | -1.81979900 | -1.21425500 |
| C | -1.57623500 | -1.80187400 | -0.13748800 |
| C | -1.17212100 | -1.89895900 | 1.18348400 |
| C | 0.19134500 | -1.99663300 | 1.40574100 |
| C | 3.82494400 | -1.87389100 | 0.39318100 |
| H | 3.87417700 | -1.07318900 | -0.34870300 |
| H | 4.13034300 | -2.79832000 | -0.09998700 |
| H | 4.54506000 | -1.65066000 | 1.18240800 |
| H | -0.47314200 | 1.43200200 | -2.43028800 |
| H | -1.88552800 | -1.87367400 | 1.99734300 |
| N | 1.54495400 | -1.97932200 | -2.10431200 |
| O | 2.53986900 | -2.66923700 | -2.02580600 |
| O | 1.23566100 | -1.34053200 | -3.09256400 |
| H | -1.04639400 | -1.74385300 | -2.23111600 |
| N | -2.99397700 | -1.62001700 | -0.42165000 |
| O | -3.35517000 | -1.62670800 | -1.58334100 |
| O | -3.75143100 | -1.45274000 | 0.51470000 |
| O | 0.56003200 | 1.12462800 | 1.90965500 |
| C | 0.12253000 | 1.07204400 | 3.26223200 |
| H | 1.01643300 | 0.90208500 | 3.85909000 |

| | | | |
|---|---|---|---|
| H | -0.34140800 | 2.01782600 | 3.55520700 |
| H | -0.58534300 | 0.25249600 | 3.41486700 |
| O | -3.95391400 | 1.53858600 | 0.52018000 |
| C | -4.93434000 | 1.46049300 | -0.50979000 |
| H | -5.89676700 | 1.45359000 | -0.00235600 |
| H | -4.87762900 | 2.32749700 | -1.17315600 |
| H | -4.81775800 | 0.53909000 | -1.08721700 |