Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

Experimental and theoretical study on the sensing mechanism of a fluorescence probe for hypochloric acid: Se···N nonbonding interaction modulating the twist process

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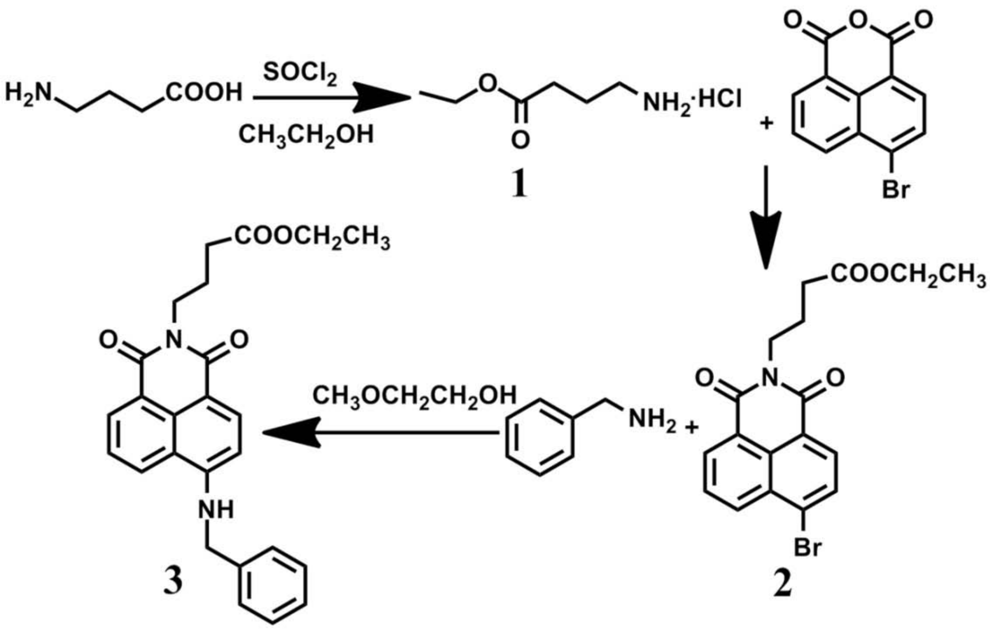
Contents:

1. Synthesis and characterization of compounds

The general synthetic route of the compound **3** was described in Scheme S1.

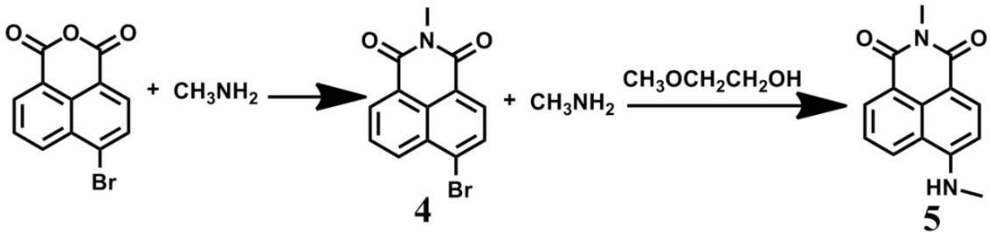


Scheme S1. The synthesis of compound 3.

Synthesis of 4-aminobutyric acid ethyl ester hydrochloride (1): This compound was prepared according to the literature procedure[1]. To 100 mL ethanol that processed with magnesium powder was added thionyl chloride (20 mL) at 0 ^oC. The solution was stirred at 0 ^oC for 30 min. After this period, 10 g (100 mmol) of 4-aminobutyric acid was added at 0 ^oC and the solution was stirred at 67 ^oC for 1 h. The volatiles were removed and the residue was washed with acetone, a white powder was obtained (8.70 g, 52.1%).

Synthesis of *N*-(butyric acid ethyl ester)-4-bromo-1,8-naphthalimide (2): This compound was prepared according to the literature procedure[2]. A mixture of 4-bromo-1,8-naphthalic anhydride (2.77g, 10 mmol), 4-aminobutyric acid ethyl ester hydrochloride **1** (2.5g, 15mmol) and triethylamine (5 mL, 35 mmol) were refluxed in ethanol (30 mL) for 6 h. The reaction mixture was concentrated in vacuo to give crude compound, which was purified by column chromatography (silica gel, CH2Cl2) to give light yellow solid (3.40 g, 87.2%). ^1H NMR (400 MHz, $CDCl_3$) δ(ppm): 8.66-8.64 (m, 1H), 8.57-8.55 (m, 1H), 8.40 (d, *J*=8.0, 1H), 8.03 (d, *J*=8.0, 1H), 7.86-7.82 (m, 1H), 4.24 (t, *J*=8.0, 2H), 4.13-4.08 (m, 2H), 2.44 (t, *J*=8.0, 2H), 2.03-2.06 (m, 2H), 1.23 (t, *J*=8.0, 3H).

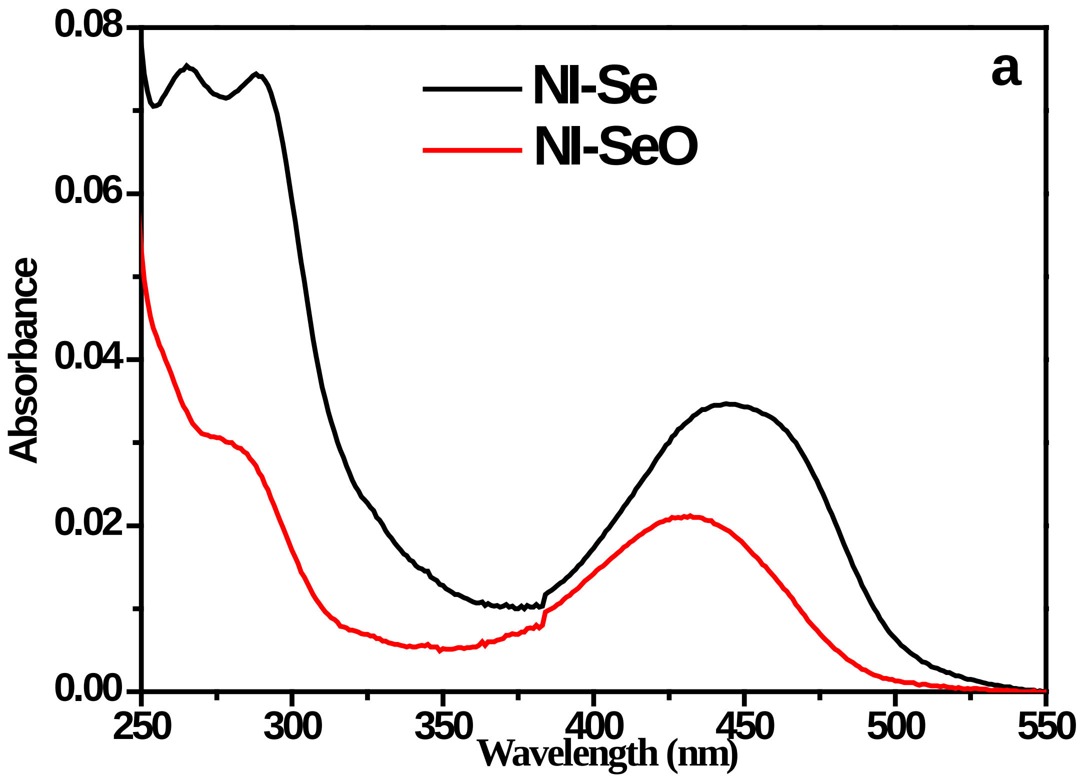
The general synthetic route of the compound **5** was described in Scheme S2.



Scheme S2. The synthesis of compound 5.

Synthesis of *N*-methyl-4-bromo-1,8-naphthalimide (4): This compound was prepared according to a slight modification of the literature procedure[3]. 5.00 g (18 mmol) of 4-bromo-1,8-naphthalic anhydride and 50 mL of 20 % methylamine aqueous solution were stirred in ethanol (30 mL) at room temperature. After this period, the mixture was filtered, and the precipitate was washed thoroughly with water. The acquired precipitate was recrystallized with ethanol to give a white solid (5.00 g, 95.0 %).

2. The absorption and excitation spectra of NI-Se and NI-SeO



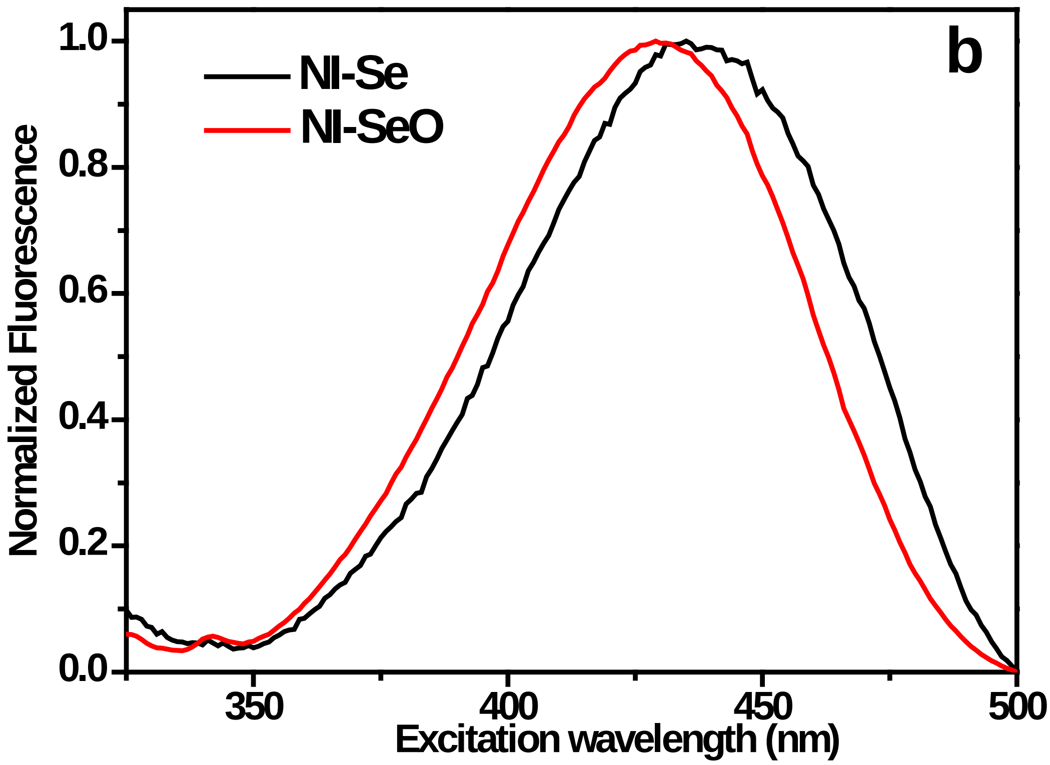
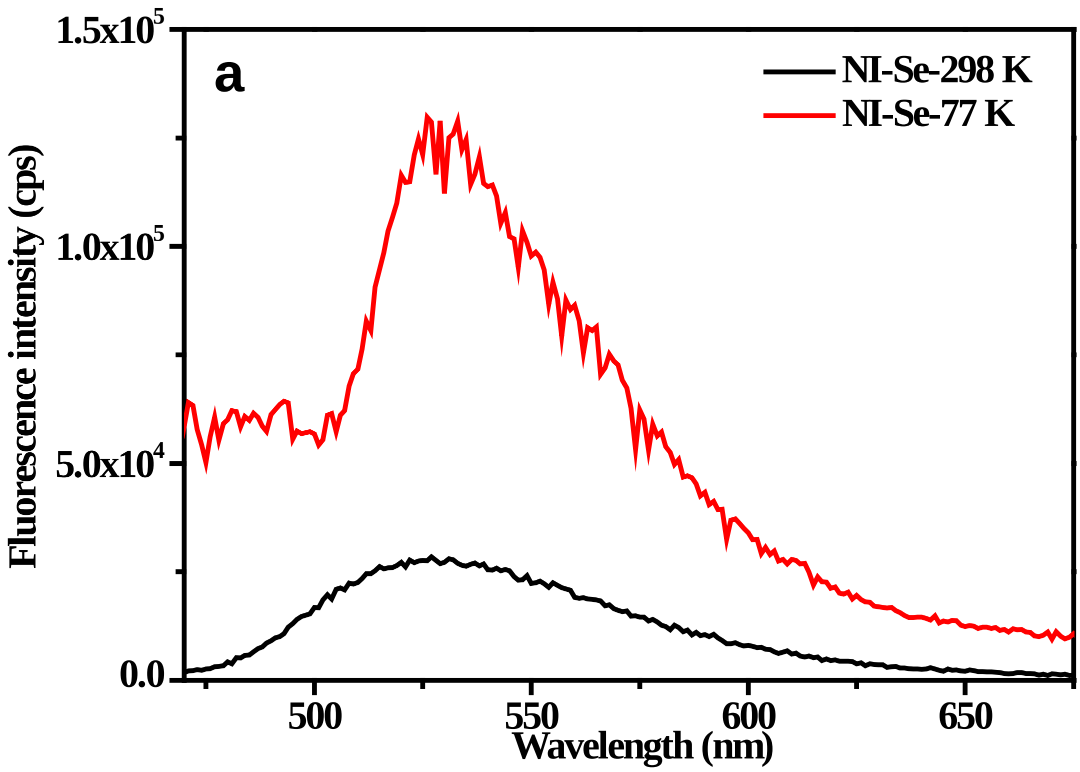


Figure S1. The absorption (a) and normalized excitation (b) spectra of NI-Se and NI-SeO at room temperature in water.

3. The fluorescence spectra of NI-Se and NI-SeO at 77K



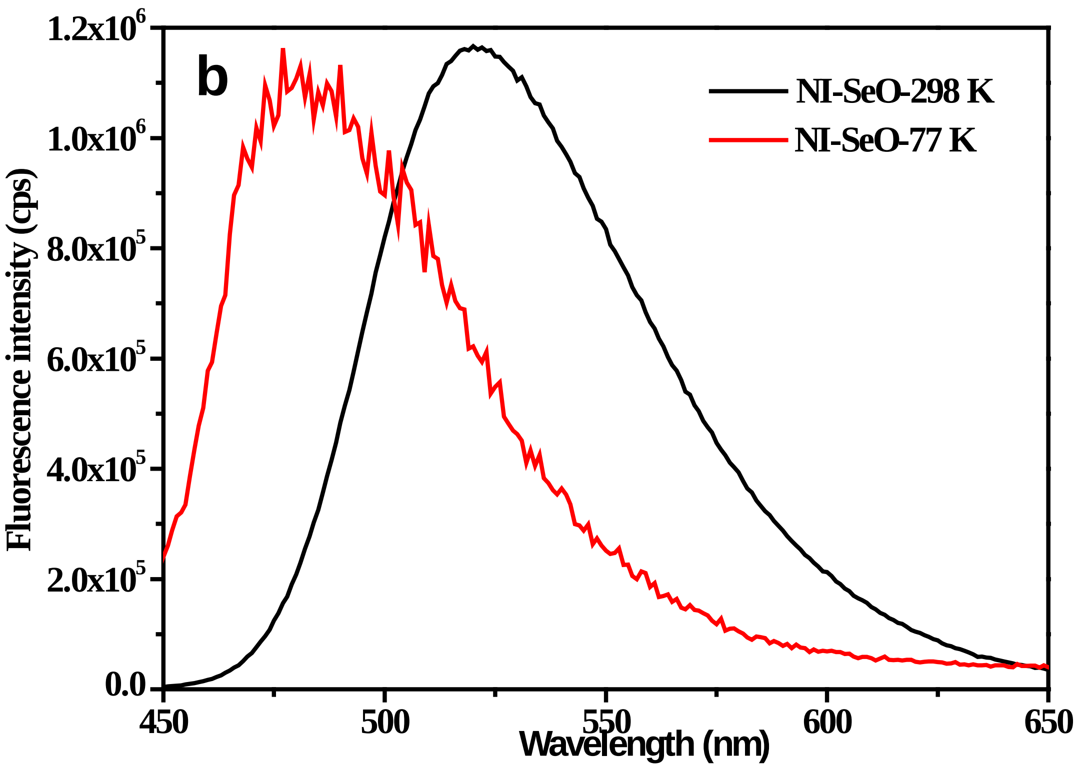


Figure S2. The fluorescence spectra of NI-Se (a) and NI-SeO (b) at 298 K and 77K in water. The excitation wavelength was set to be 420 nm for NI-SeO. The result was reproduced from Ref. 5 with permission from The Royal Society of Chemistry.

4. The fluorescecne quantum yields of NI-Se and NI-SeO in different solvents

The quantum yields of NI-Se and NI-SeO in different solvents were measured with the solution of fluorescein in 0.1 M NaOH (ϕ = 0.95) as a fluorescence standard[4]. The quantum yields of NI-Se and NI-SeO in water were taken from reference 5 (Z. Lou, P. Li, Q. Pan and K. Han, *Chem. Commun.*, 2013, **49**, 2445-2447.)

Table S1. The quantum yields of NI-Se in different solvents.

Solvent	*n*-hexane	CH_2Cl_2	CH_3CN	CH_3CH_2OH	CH_3OH	H_2O
Quantum Yield	0.53	0.50	0.39	0.26	0.17	0.04

Table S2. The quantum yields of NI-SeO in different solvents.

Solvent	*n*-hexane	CH_2Cl_2	CH_3CN	CH_3CH_2OH	CH_3OH	H_2O
Quantum Yield	0.27	0.48	0.44	0.46	0.42	0.45

5. The optimized geometry of NI-Se in ICT state

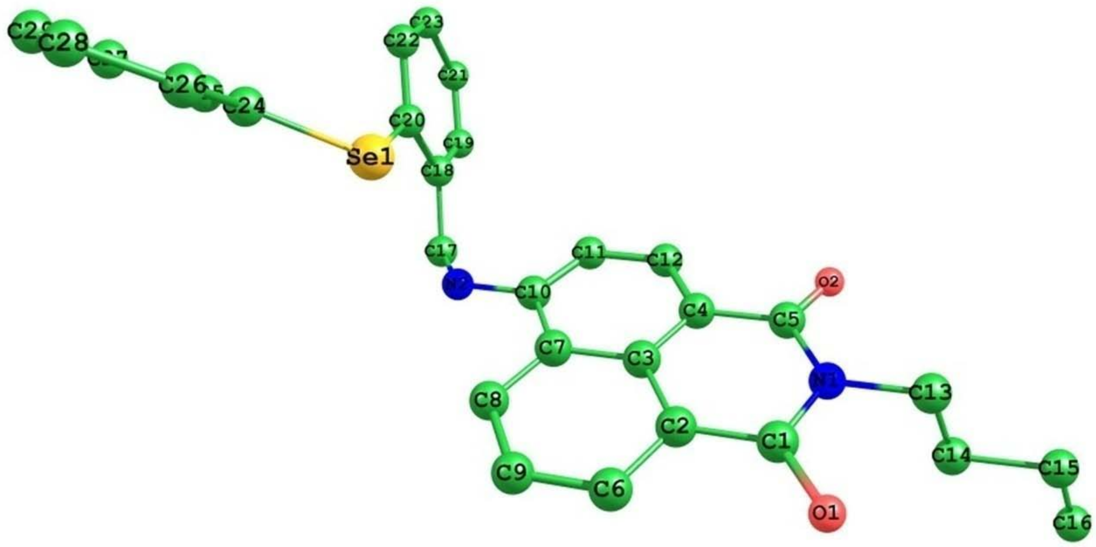


Figure S3. Structures of NI-Se in ICT state were optimized with the dihedral angle C10-N2-C17-C18 fixed. Green: C; red: O; blue: N; yellow: Se; H atoms have been hidden for simplicity.

6. The relevant molecular orbitals of NI-SeO

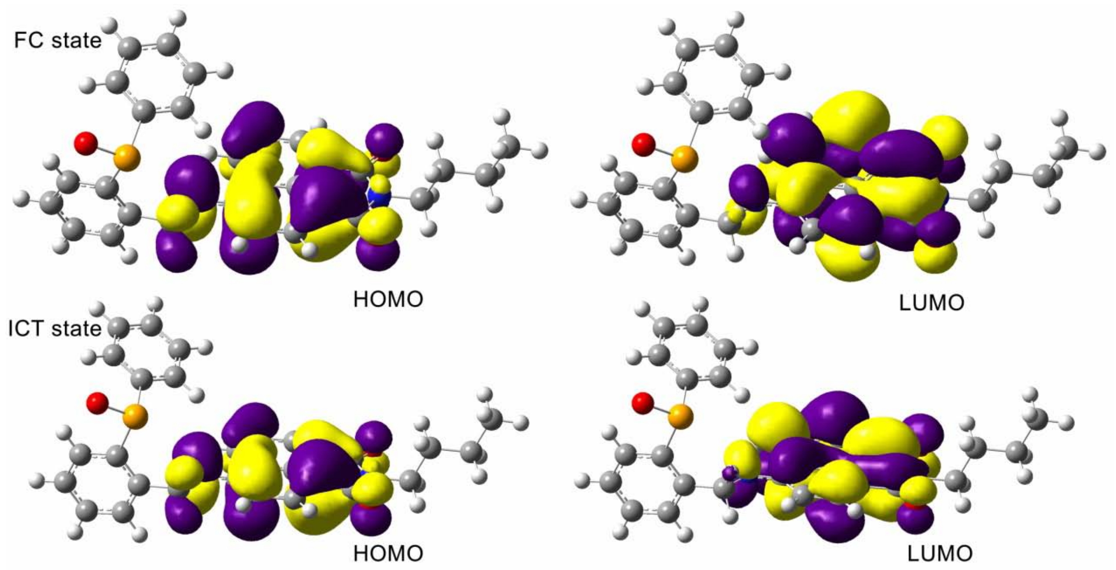


Figure S4. The relevant frontier molecular orbitals NI-SeO.

7. The measurements of wavelength in ICT and TICT state

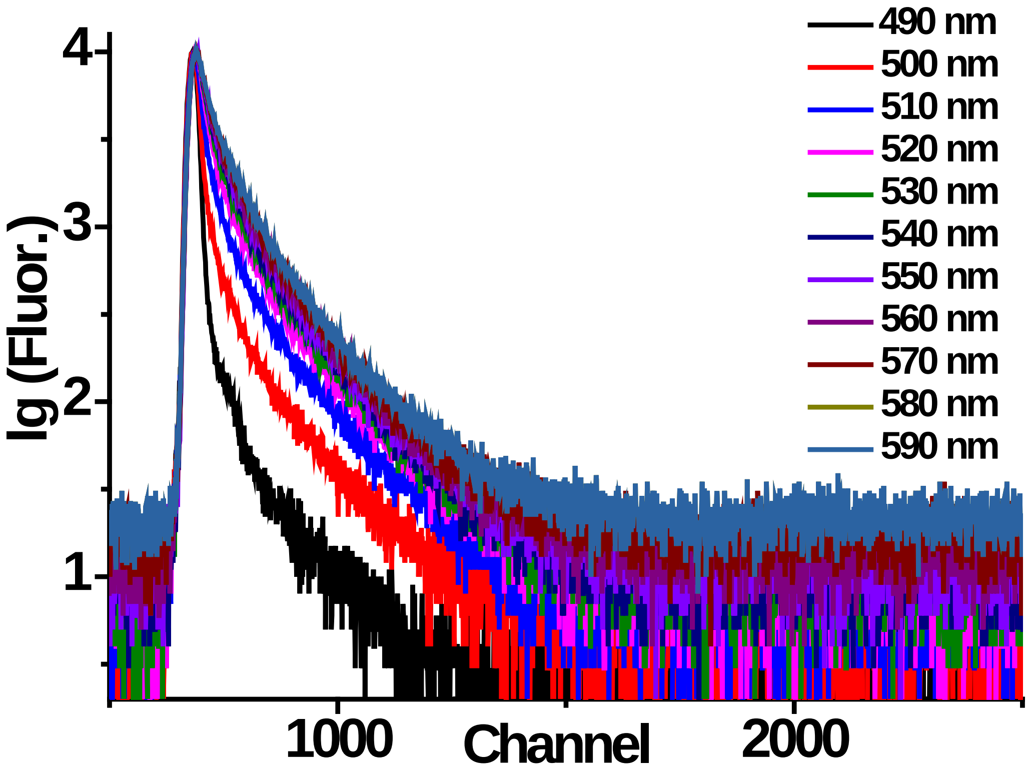


Figure S5. Fluorescence decays of NI-Se probed at different wavelength in water (298 K) from time-correlated single photon counting (TCSPC) data.

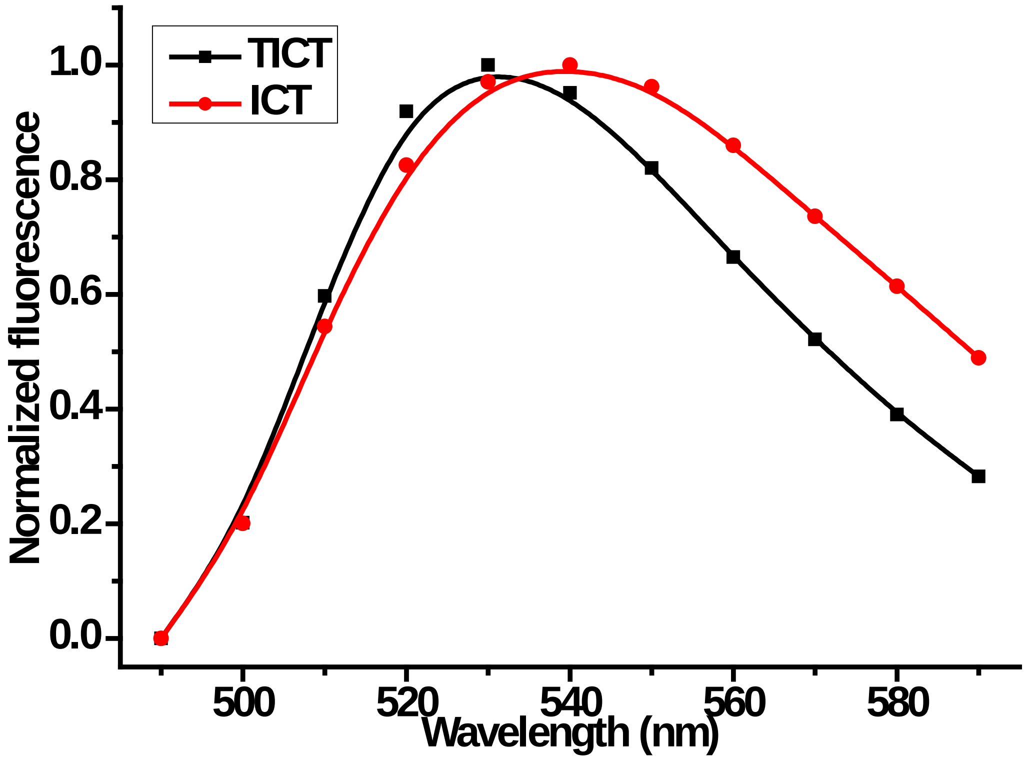


Figure S6. Normalized fluorescence of ICT and TICT state at different wavelength in water (298 K). The fluorescence intensity: $f_i = F_i \times A_i$, where f is the fluorescence intensity of ICT or TICT state; F is the fluorescence intensity of NI-Se; A is the component of the ICT or TICT obtained from the global fitting of the fluorescence decays of NI-Se with three exponents; i represents different wavelength.

8. The influences of viscosity on emission spectra

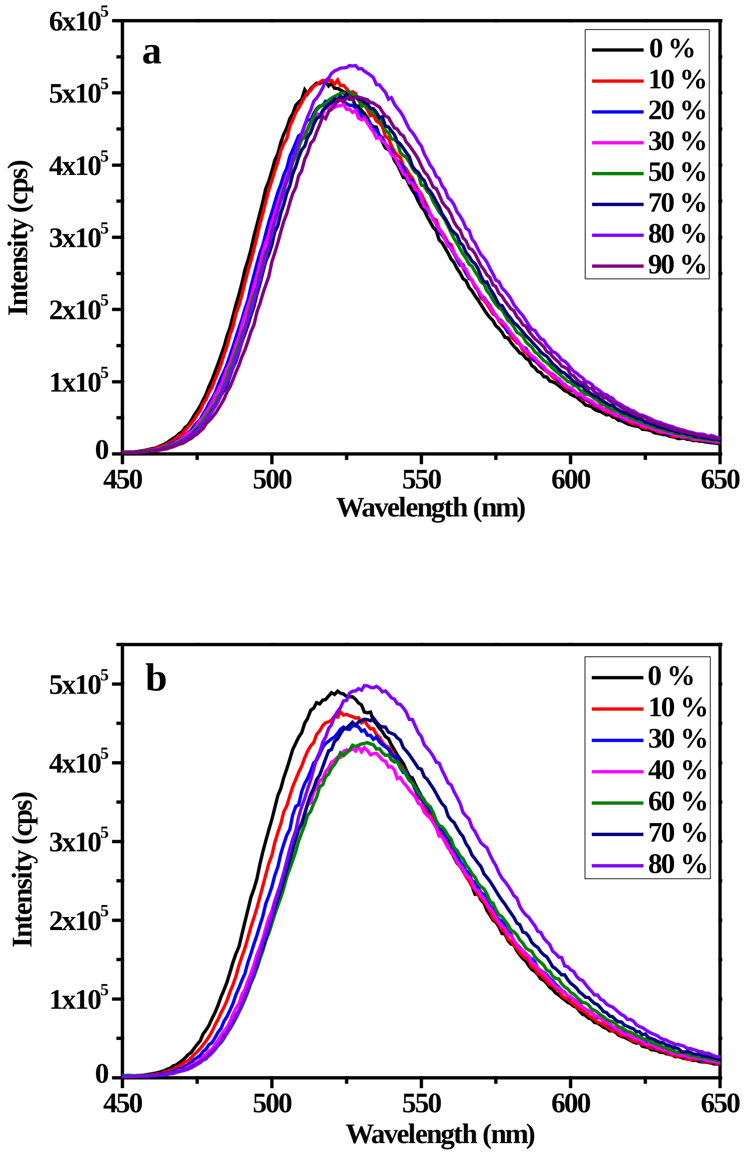
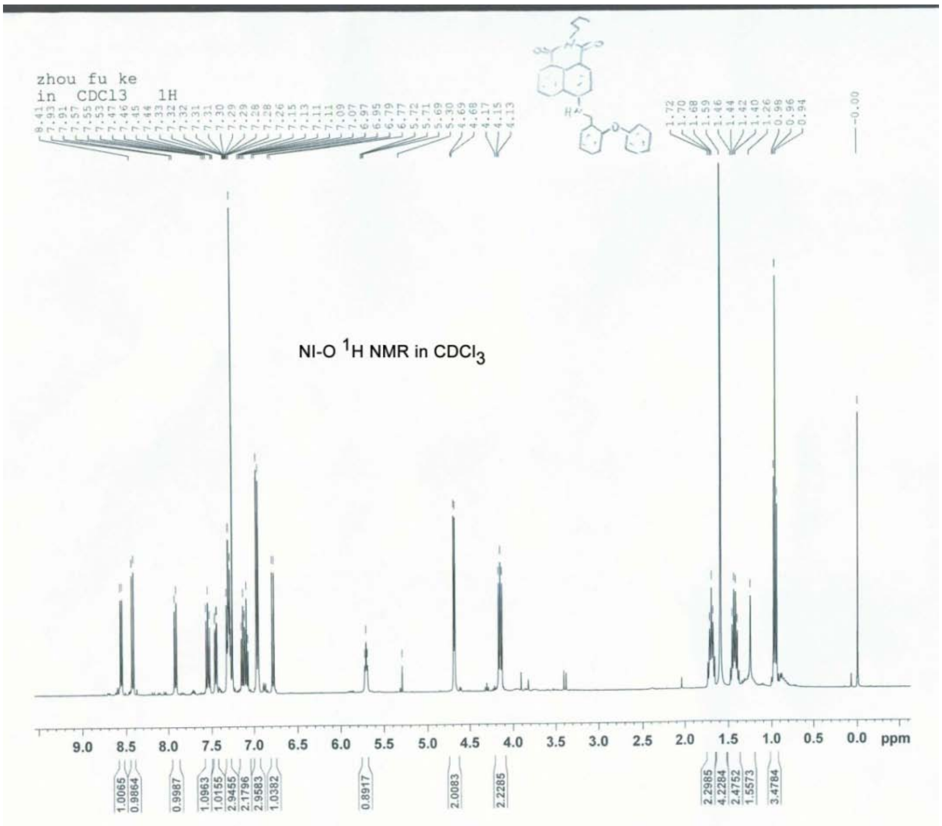
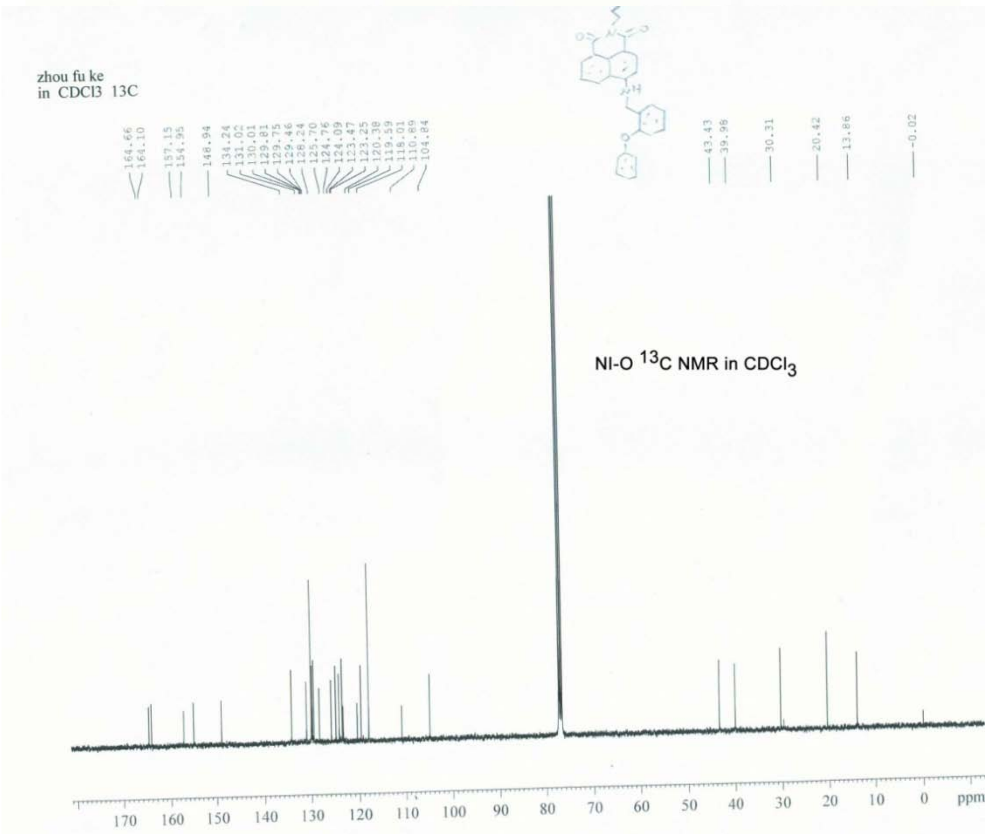
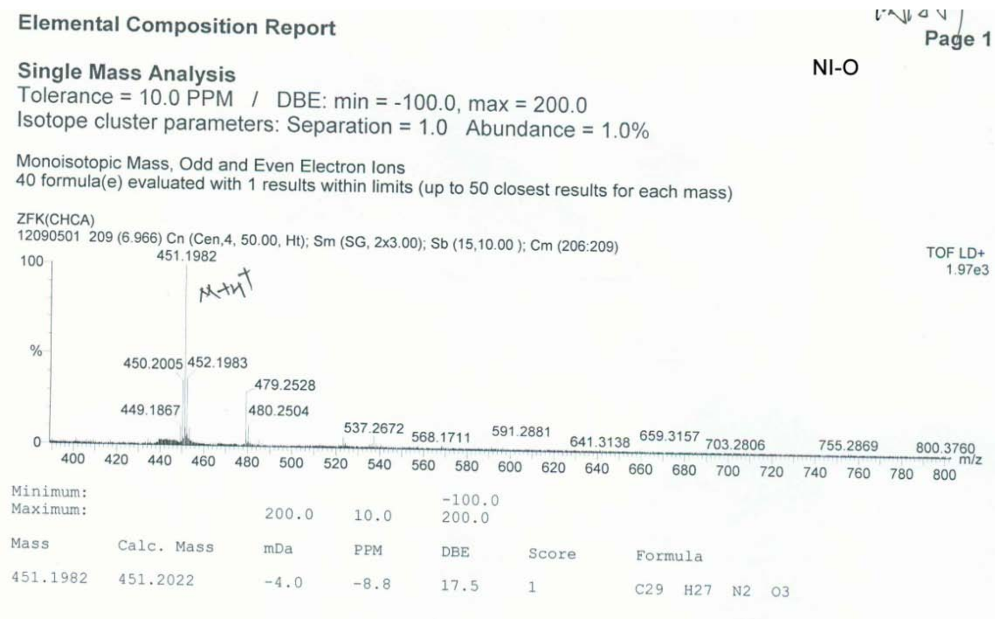


Figure S7. The fluorescence spectra of compound **3** (a) and **5** (b) (3.0 μM) in ethanol upon the addition of glycerin. The fluorescence intensity was measured with the excitation wavelength 435 nm, and the excitation and emission slits set to 2 and 1 nm, respectively.

9. Additional spectroscopic data







Elemental Composition Report

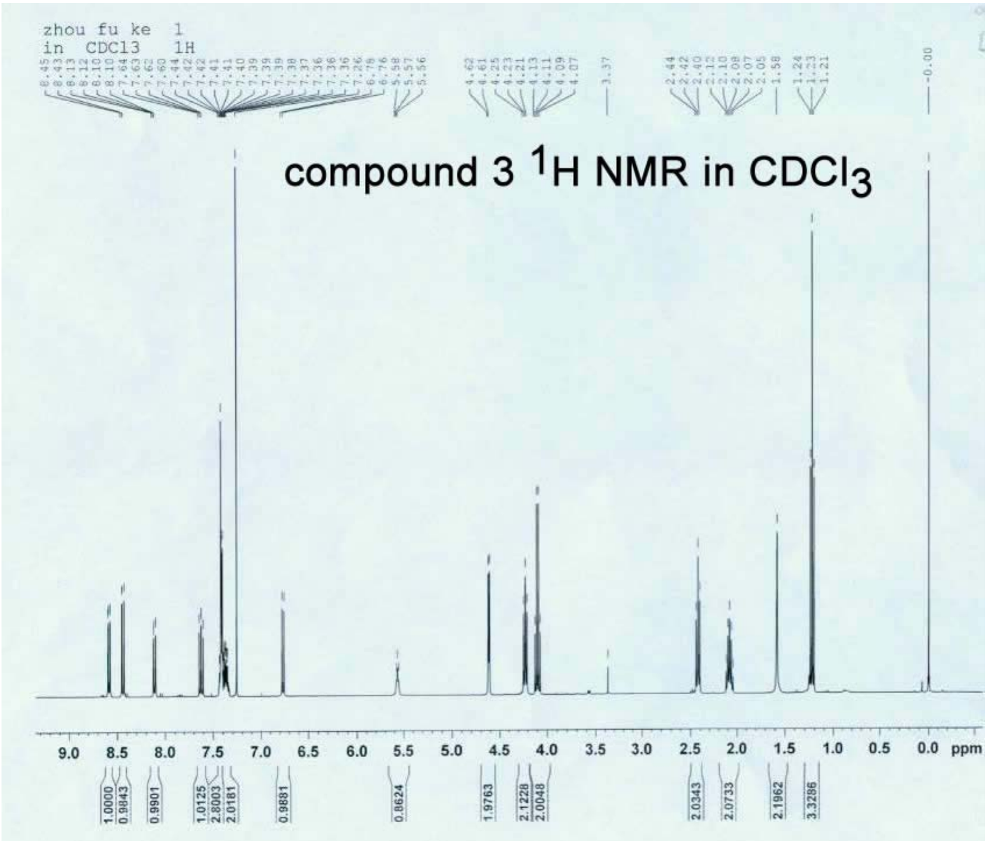
Page 1

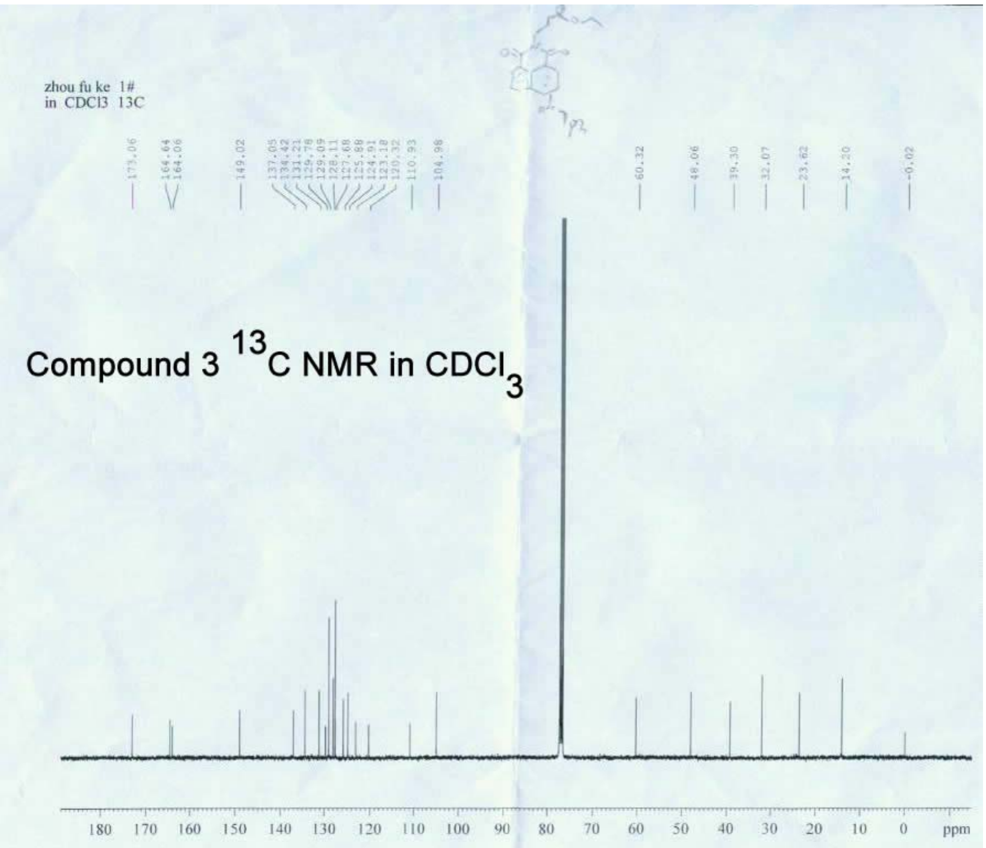
NI-O

Single Mass Analysis
Tolerance = 10.0 PPM / DBE: min = -100.0, max = 200.0
Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

Monoisotopic Mass, Odd and Even Electron Ions
40 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Minimum:				-100.0		
Maximum:		200.0	10.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
451.1982	451.2022	-4.0	-8.8	17.5	1	C29 H27 N2 O3





Single Mass Analysis

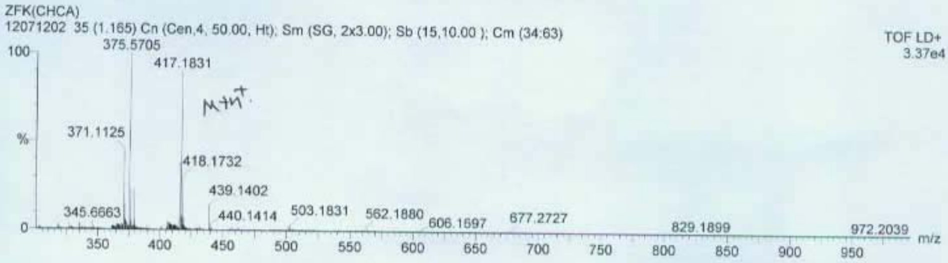
Tolerance = 10.0 PPM / DBE: min = -100.0, max = 200.0

Isotope cluster parameters: Separation = 1.0 Abundance = 1.0%

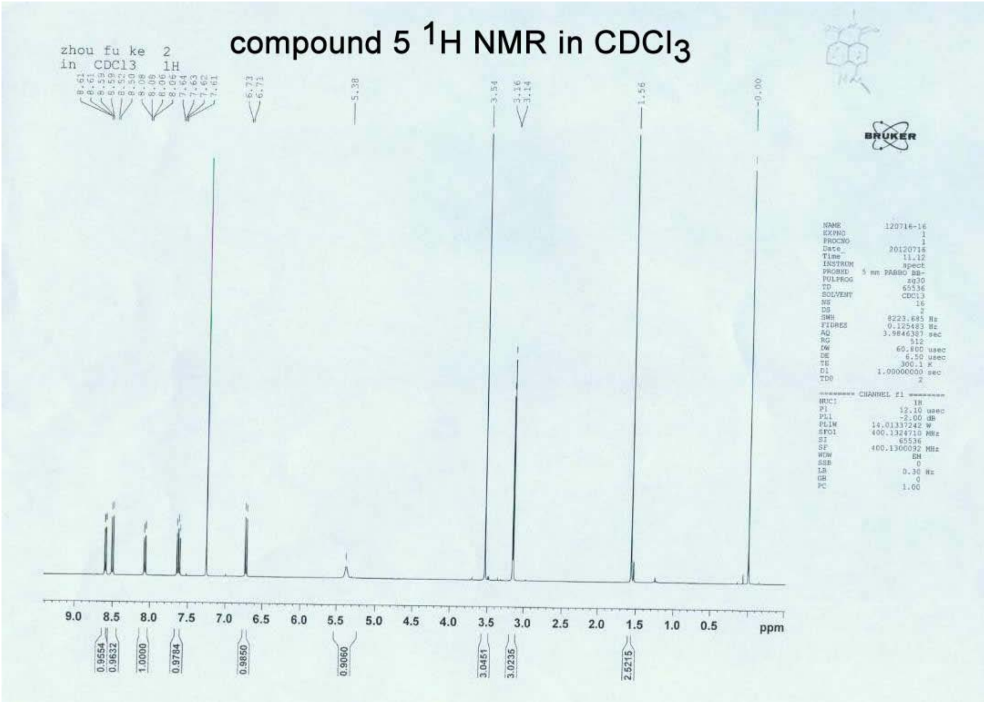
compound 3

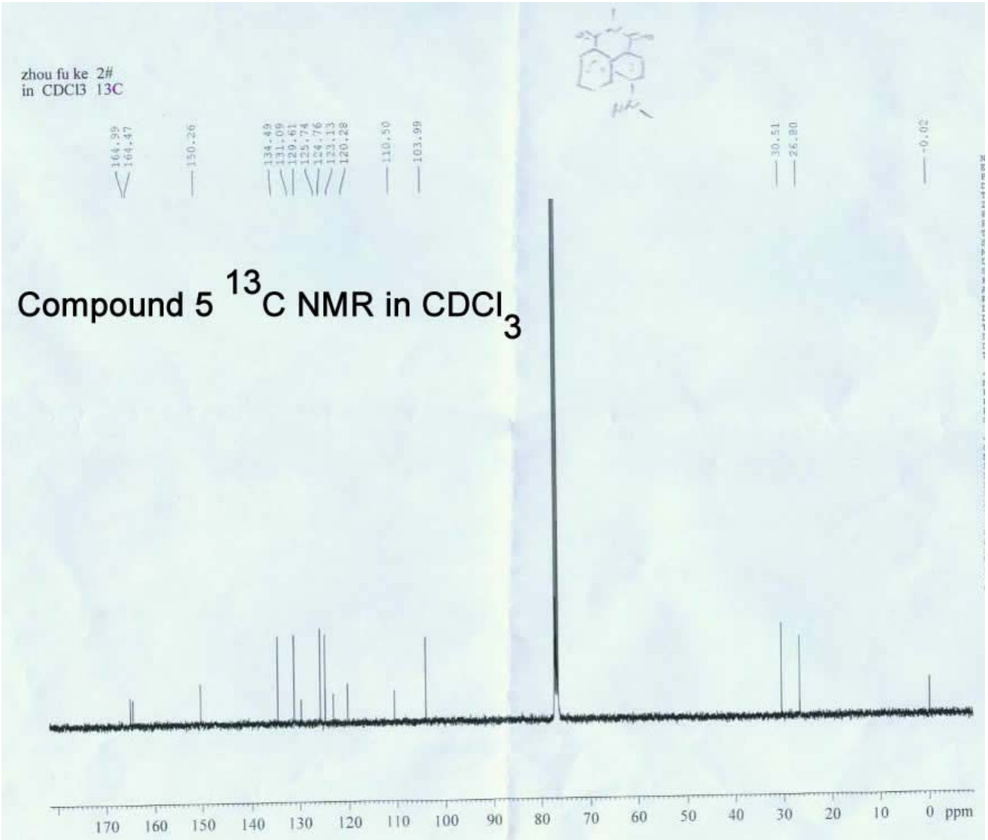
Monoisotopic Mass, Odd and Even Electron Ions

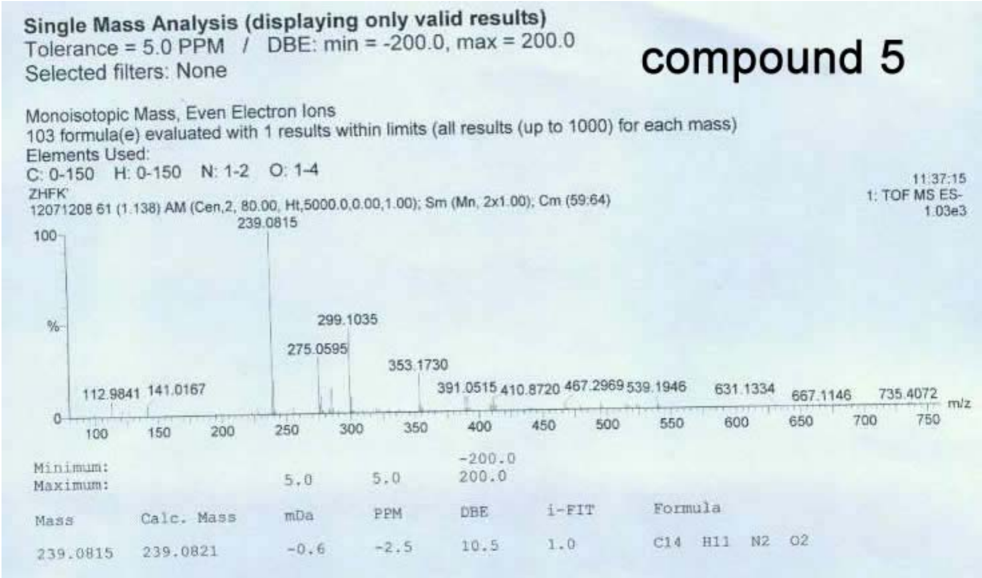
19 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)



Minimum:				-100.0		
Maximum:		200.0	10.0	200.0		
Mass	Calc. Mass	mDa	PPM	DBE	Score	Formula
417.1831	417.1814	1.7	4.0	14.5	1	C25 H25 N2 O4


compound 5 ^{1}H NMR in $CDCl_3$
zhou fu ke 2
in CDCl3 1H
ppm


Compound 5 ^{13}C NMR in $CDCl_3$
zhou fu ke 2#
in CDCl3 13C
ppm



10. References

1. Y.-M. Lin and M. J. Miller, *The Journal of Organic Chemistry*, 2001, **66**, 8282-8285.
2. J. Wu, T. Yi, T. Shu, M. Yu, Z. Zhou, M. Xu, Y. Zhou, H. Zhang, J. Han, F. Li and C. Huang, *Angewandte Chemie International Edition*, 2008, **47**, 1063-1067.
3. P. Yang, Q. Yang and X. Qian, *Tetrahedron*, 2005, **61**, 11895-11901.
4. J. H. Brannon and D. Magde, *The Journal of Physical Chemistry*, 1978, **82**, 705-709.
5 Z. Lou, P. Li, Q. Pan and K. Han, *Chemical Communications*, 2013, **49**, 2445-2447.

11. Cartesian coordinates for the optimized structures

Optimized S_0 state of NI-Se

C	-4.80607200	-1.22824500	-0.75162000
C	-3.37282700	-1.52996200	-0.56412000
C	-2.49829600	-0.54060400	-0.05266600
C	-2.99972800	0.74222700	0.27325200
C	-4.40739300	1.06571600	0.09048300
C	-2.89817000	-2.78869900	-0.88917500
C	-1.11676200	-0.85117700	0.12414300
C	-0.67504600	-2.14357200	-0.22580600
C	-1.54505400	-3.09435200	-0.72128100
C	-0.23010600	0.16981500	0.65393200
C	-0.77282600	1.42750200	0.95768300
C	-2.12037600	1.69507800	0.77419200
H	-2.49962200	2.67728700	1.02530300

H	-0.13969100	2.20863400	1.34879500
H	-3.58386900	-3.53085300	-1.27544700
H	-1.17706700	-4.07843500	-0.98088700
O	-5.60272400	-2.06394600	-1.17521800
O	-4.89257100	2.16423800	0.36629800
N	-5.23623800	0.05623900	-0.43264500
C	-6.66548800	0.37044800	-0.62560900
C	-7.51555100	0.06070900	0.60762800
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C	-8.99405700	0.38280000	0.37926800
H	-7.40613300	-0.99696200	0.86468100
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H	-9.09603200	1.43998300	0.11181800
H	-9.35913800	-0.18961100	-0.48017500
C	-9.86330400	0.07961300	1.60043500
H	-10.91176800	0.31968900	1.40947100
H	-9.80652000	-0.97847900	1.87025500
H	-9.53956300	0.66182300	2.46744000
H	0.36466200	-2.42266100	-0.11611100
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H	2.89313700	0.22642300	1.75905500
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N	1.07645800	-0.11412800	0.86330100
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C	2.46126100	3.03146300	0.12760900
C	3.53423700	1.10942900	-0.83275200
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C	7.24880500	-2.27046600	1.19974600
H	5.65944600	-3.00995100	-0.03763700
C	7.83467700	-1.15409900	1.79418900
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H	7.67900900	-3.25429200	1.34489800
H	8.72282200	-1.26349300	2.40418800
H	1.42446700	-1.01227900	0.56947500

Optimized TICT state of NI-Se

C	-4.30883400	-1.56480800	0.37032400
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C	-1.92955900	-1.25292600	-0.27252800
C	-2.31161200	-0.23694100	-1.18848200
C	-3.71780300	0.14024300	-1.33029000
C	-2.52824600	-2.92197900	1.42193000
C	-0.55373200	-1.60472900	-0.12534500
C	-0.20195500	-2.61256900	0.81394600
C	-1.19222100	-3.25140400	1.56331500
C	0.40976300	-0.92151400	-0.93535500
C	-0.00220800	0.07029700	-1.83552700
C	-1.34093300	0.41297000	-1.95803200
H	-1.64151100	1.18219800	-2.65500700
H	0.72318500	0.57578200	-2.45662800
H	-3.28541100	-3.42305100	2.00843800
H	-0.90361100	-4.01877400	2.27237700
O	-5.22673200	-2.10634300	1.02377400
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H	2.77380700	-1.26898100	-2.63394100
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C	5.19804800	-1.55795700	-1.77765500

C	4.45157000	-0.59048400	0.28261600
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Optimized ICT state of NI-Se

C	-4.37009000	-1.54728100	-0.14927600
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C	-2.60414100	-2.90573000	0.92493100
C	-0.88314100	-0.65640100	1.03786000
C	-0.46811200	-1.92715300	1.51949500
C	-1.33349800	-3.02169600	1.45863400
C	-0.06046100	0.51307600	1.09977900
C	-0.51888900	1.72917000	0.57582200
C	-1.78238000	1.83503600	0.01715500
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H	0.11467100	2.60414000	0.60869500
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H	2.73867000	1.20284400	2.77470600
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C	2.79794700	2.17397900	0.87562700
C	3.03109300	3.55073800	0.88564100
C	3.35265100	1.42348700	-0.16825200
C	3.79402200	4.16288100	-0.10172800
H	2.60663400	4.14668500	1.68529600
C	4.11012300	2.03413600	-1.17291900
C	4.33456700	3.40325200	-1.13593300
H	3.96155800	5.23218700	-0.06639800
H	4.51533400	1.44400300	-1.98432100
H	4.91950500	3.87257900	-1.91678200
Se	2.98928500	-0.46794300	-0.33253000
C	4.76509500	-1.17886600	-0.48712200
C	5.88976200	-0.56350900	0.07283300
C	4.87491200	-2.42174400	-1.12502100
C	7.12740900	-1.18353000	-0.03635500
H	5.80281500	0.38447500	0.58591400
C	6.11916400	-3.02984900	-1.22641300
H	4.00096000	-2.89996800	-1.55051400
C	7.24602400	-2.41357600	-0.68380900
H	8.00123000	-0.70933400	0.39286300
H	6.20877000	-3.98414000	-1.73004300
H	8.21444300	-2.89142900	-0.76251300
H	1.34320100	-0.38654800	2.26797700

Optimized S_0 state of NI-SeO

C	-4.76187100	-0.00687100	1.36274500
C	-3.31400300	-0.05035000	1.65019800
C	-2.42276400	-0.64357500	0.72367700

C	-2.92197300	-1.20368100	-0.47705000
C	-4.34686200	-1.18073100	-0.77783700
C	-2.84041200	0.49801100	2.82944000
C	-1.02711800	-0.66992200	1.01588900
C	-0.58720100	-0.10375200	2.22941900
C	-1.47367800	0.46867900	3.11987500
C	-0.12481900	-1.27673800	0.05601600
C	-0.66247200	-1.81532700	-1.12289100
C	-2.02631900	-1.77601000	-1.37249200
H	-2.40581200	-2.20122400	-2.29273500
H	-0.00973900	-2.26572800	-1.85627700
H	-3.53841800	0.94743100	3.52296400
H	-1.10845900	0.89603800	4.04464400
O	-5.56767500	0.51581700	2.13042400
O	-4.82930300	-1.64911300	-1.81001800
N	-5.19592100	-0.58984700	0.17564900
C	-6.64228700	-0.55809300	-0.11810700
C	-7.06519400	0.68954900	-0.89535000
H	-7.16299700	-0.60577500	0.83512500
H	-6.87278600	-1.45549900	-0.68685500
C	-8.56916700	0.70444400	-1.17841100
H	-6.79038100	1.58136700	-0.32434600
H	-6.51357000	0.72995500	-1.83908200
H	-8.84102900	-0.20034700	-1.73256000
H	-9.11497800	0.66111200	-0.22989000
C	-9.01270600	1.93760800	-1.96669900
H	-10.08946400	1.92370800	-2.15053000
H	-8.77823600	2.85688100	-1.42312700
H	-8.50888500	1.98633200	-2.93583700
H	0.46253300	-0.10513300	2.49306200
C	2.19123300	-1.91007900	-0.59945500
H	2.19595700	-1.37224500	-1.55217200
H	1.90993000	-2.94331500	-0.81917400
N	1.20288600	-1.32282900	0.30280100
C	3.56087100	-1.90422500	0.04064600
C	3.86153400	-2.89076900	0.98664700
C	4.55093400	-0.96032600	-0.24679200
C	5.09875100	-2.93326700	1.61785200
H	3.11101900	-3.63773900	1.21887100
C	5.79867800	-1.00263400	0.36311200
C	6.07220700	-1.98801300	1.30516200
H	5.30666900	-3.70983100	2.34355200
H	6.55139800	-0.27425800	0.08732700
H	7.04268300	-2.02069000	1.78492600

Se	4.30397000	0.44351100	-1.62996500
C	3.63845700	1.88177200	-0.45944300
C	4.55070500	2.69627800	0.19819900
C	2.26796400	2.09798600	-0.37026000
C	4.07445000	3.74132000	0.98568700
H	5.61426300	2.52271300	0.09083300
C	1.80201000	3.14577700	0.42183700
H	1.56798100	1.46592400	-0.90346200
C	2.70313100	3.96433800	1.09833400
H	4.77487100	4.38265000	1.50674500
H	0.73692200	3.32531600	0.50086300
H	2.33749000	4.78078900	1.70898500
H	1.56374200	-0.88158200	1.13191600
O	5.88986200	0.91006300	-1.94212800

Optimized ICT state of NI-SeO

C	-4.79588100	0.21397000	1.35371200
C	-3.38326900	0.19005400	1.62137500
C	-2.49054600	-0.51797500	0.77186900
C	-3.01033900	-1.22309600	-0.35003000
C	-4.45770200	-1.20086200	-0.64426200
C	-2.85778200	0.88613400	2.74392000
C	-1.09884600	-0.53635100	1.04546800
C	-0.60926800	0.16074400	2.17840300
C	-1.50168500	0.85908700	3.00263400
C	-0.24586000	-1.27006500	0.13979900
C	-0.80731200	-1.96834100	-0.96987600
C	-2.15929700	-1.94121000	-1.20985200
H	-2.57940000	-2.46664500	-2.05456600
H	-0.15890300	-2.51597700	-1.63802100
H	-3.53298400	1.42971900	3.38913200
H	-1.11253600	1.38893000	3.86406800
O	-5.62046900	0.82718900	2.05900400
O	-4.91382800	-1.78839200	-1.63361300
N	-5.26730500	-0.50764600	0.22300800
C	-6.71517200	-0.48327100	-0.05578900
C	-7.12972500	0.68066600	-0.95787800
H	-7.22322600	-0.41715000	0.90283200
H	-6.96942100	-1.43281400	-0.52181400
C	-8.63604800	0.68739400	-1.22864500
H	-6.83789100	1.62258300	-0.48417400
H	-6.58667800	0.61638300	-1.90547100
H	-8.92349400	-0.26163100	-1.69380200
H	-9.17301700	0.73859900	-0.27541400

C	-9.07353700	1.84738100	-2.12410300
H	-10.15144900	1.82690900	-2.30051000
H	-8.82778700	2.81023100	-1.66800000
H	-8.57491300	1.80285400	-3.09613500
H	0.43958900	0.16291300	2.43751900
C	2.07275800	-2.00427900	-0.46724300
H	2.09798200	-1.57333100	-1.47152400
H	1.75778100	-3.04447600	-0.57053500
N	1.08274100	-1.28934400	0.34293300
C	3.43045900	-1.96532600	0.19418900
C	3.69242100	-2.87479600	1.22558600
C	4.44454400	-1.07079000	-0.16002300
C	4.91909100	-2.89084500	1.87719700
H	2.92117900	-3.58258200	1.50707800
C	5.68206500	-1.09044100	0.47343100
C	5.91859900	-1.99763300	1.49951100
H	5.09863100	-3.60622800	2.67007300
H	6.45954000	-0.40746100	0.15414400
H	6.88100900	-2.01004600	1.99606600
Se	4.24294100	0.21405400	-1.66085100
C	3.89247300	1.82820700	-0.58587500
C	4.95812100	2.64621100	-0.23784000
C	2.58163800	2.15081700	-0.25232200
C	4.70526900	3.80672000	0.49034800
H	5.96557900	2.38384600	-0.53605500
C	2.34050600	3.31272800	0.47753700
H	1.75702600	1.51368100	-0.54914100
C	3.40013600	4.13774600	0.84880300
H	5.52784900	4.45259500	0.77253200
H	1.32485100	3.57478000	0.74732000
H	3.20782500	5.04214000	1.41294600
H	1.45636200	-0.74480700	1.10791800
O	5.83349000	0.43153000	-2.16156500

Optimized S_0 state of NI-O

C	4.11312800	-1.44370700	0.55598300
C	2.71680300	-1.63160500	0.11390000
C	1.91957500	-0.50990200	-0.21953000
C	2.46159400	0.79402300	-0.12380700
C	3.83505100	1.00461200	0.30953400
C	2.20122500	-2.91295700	0.02431100
C	0.57369600	-0.71061800	-0.64817700
C	0.08929400	-2.03196000	-0.72500900
C	0.88338500	-3.11239400	-0.39538600

C	-0.23463900	0.44591600	-0.99140800
C	0.34318000	1.71920600	-0.86974300
C	1.65575600	1.87783300	-0.45376100
H	2.06586500	2.87669000	-0.37820000
H	-0.23606500	2.59931800	-1.10249900
H	2.82797900	-3.75630700	0.28145200
H	0.48398200	-4.11589700	-0.46372600
O	4.84358000	-2.39039400	0.84389900
O	4.35555900	2.11798300	0.39823500
N	4.58664400	-0.13791400	0.64156300
C	5.98051400	0.06045200	1.08472700
C	6.98183000	0.04403300	-0.07164300
H	6.20691500	-0.73197800	1.79409700
H	6.01700600	1.01486700	1.60384100
C	8.41832900	0.25069000	0.41375800
H	6.90667600	-0.91032900	-0.60105500
H	6.71919100	0.82914900	-0.78670200
H	8.48340500	1.20186700	0.95282400
H	8.67059800	-0.53193100	1.13724700
C	9.43805600	0.23966300	-0.72595400
H	10.45283700	0.39025100	-0.35052900
H	9.41809000	-0.71305200	-1.26209200
H	9.22809600	1.03268500	-1.44880900
H	-0.92350200	-2.23190800	-1.04956800
C	-2.45661600	1.33596200	-1.75180600
H	-3.17975300	0.89550900	-2.43880400
H	-1.95139800	2.13603000	-2.29147200
N	-1.49997000	0.27622900	-1.43724700
C	-3.18128700	1.91014700	-0.55040900
C	-3.01530500	3.24069800	-0.16816000
C	-4.06627400	1.11697900	0.19183600
C	-3.69641200	3.77246900	0.92410900
H	-2.34643600	3.87110800	-0.74307600
C	-4.74567200	1.63003200	1.29256300
C	-4.55883200	2.96127900	1.65419000
H	-3.55328100	4.80943000	1.20093200
H	-5.41640100	0.99737900	1.85862100
H	-5.08868300	3.35804800	2.51162800
C	-5.36067900	-0.90456600	0.01332200
C	-6.57306000	-0.42880000	-0.47906000
C	-5.27916600	-2.13735600	0.64965700
C	-7.71900200	-1.20156600	-0.31883700
H	-6.61710200	0.52879000	-0.98225600
C	-6.43206300	-2.90518200	0.79773300

H	-4.32247700	-2.48500400	1.01870600
C	-7.65374900	-2.43972400	0.31849700
H	-8.66420200	-0.83640300	-0.70196500
H	-6.37188100	-3.86704400	1.29225400
H	-8.54871100	-3.03773700	0.43715600
H	-1.89273200	-0.64997400	-1.41708600
O	-4.17497300	-0.20805200	-0.19334700

Optimized S_1 state of NI-O

C	4.09496900	-1.41710200	0.62140100
C	2.71965700	-1.57895000	0.23770900
C	1.93311600	-0.46079500	-0.15090000
C	2.52372700	0.83535400	-0.15913600
C	3.93970800	1.01704200	0.22148200
C	2.12518800	-2.87093900	0.23682000
C	0.57517900	-0.62791300	-0.52069200
C	0.01119100	-1.93050400	-0.50315000
C	0.80163300	-3.02349700	-0.12733600
C	-0.17251900	0.54811000	-0.90240100
C	0.46014500	1.82607700	-0.90397500
C	1.77762800	1.96370900	-0.53818600
H	2.24947300	2.93515400	-0.53992800
H	-0.10092400	2.70183400	-1.19256400
H	2.72056900	-3.72515000	0.52568200
H	0.35851200	-4.01245000	-0.12280700
O	4.83184700	-2.36202800	0.96520100
O	4.46656800	2.13667400	0.19524600
N	4.63657100	-0.10147700	0.60868000
C	6.04564800	0.06756400	1.00758600
C	7.01844300	-0.04813100	-0.16742400
H	6.25972300	-0.69636800	1.75062600
H	6.13246100	1.04575200	1.47592400
C	8.47266200	0.13113300	0.27436400
H	6.89602900	-1.02746600	-0.63928200
H	6.76791800	0.70459900	-0.92083400
H	8.58711000	1.11107000	0.75005000
H	8.71025000	-0.61358000	1.04163600
C	9.46530200	0.00534400	-0.88221100
H	10.49364700	0.13687700	-0.53776600
H	9.39434000	-0.97798600	-1.35493900
H	9.27155200	0.75852200	-1.65083900
H	-1.01813800	-2.11057500	-0.77764600
C	-2.41907700	1.46634900	-1.61683500
H	-3.08555600	1.03016800	-2.36117000

H	-1.90029700	2.29797700	-2.08505400
N	-1.46041600	0.41605600	-1.26673100
C	-3.21709300	1.95340300	-0.42402100
C	-3.05164500	3.24214300	0.07945000
C	-4.15291500	1.11035100	0.19022300
C	-3.79900600	3.69201400	1.16476700
H	-2.33470900	3.90290300	-0.39409300
C	-4.90114800	1.54476600	1.28025600
C	-4.72060400	2.83816800	1.76234500
H	-3.66256700	4.69928000	1.53747500
H	-5.61420700	0.88042700	1.74937300
H	-5.30256400	3.17222700	2.61263900
C	-5.39619200	-0.92388800	-0.14138000
C	-6.60840600	-0.49456200	-0.67311400
C	-5.28426300	-2.15133100	0.49898000
C	-7.72793300	-1.31129500	-0.54801200
H	-6.67144400	0.46062000	-1.17915400
C	-6.41054800	-2.96360400	0.61181400
H	-4.32639900	-2.46073000	0.89770000
C	-7.63338600	-2.54544600	0.09351900
H	-8.67440900	-0.98414700	-0.96093500
H	-6.32893600	-3.92250200	1.10887400
H	-8.50751100	-3.17812000	0.18479700
H	-1.86528300	-0.50837700	-1.21488200
O	-4.23572500	-0.17257600	-0.31397100