

X-Ray Diffraction, Spectroscopy, Optical Properties, NPA, NBO, FMO, and Hirshfeld Surface Analyses of Two Newly Synthesized Piperidinium Ionic Liquids

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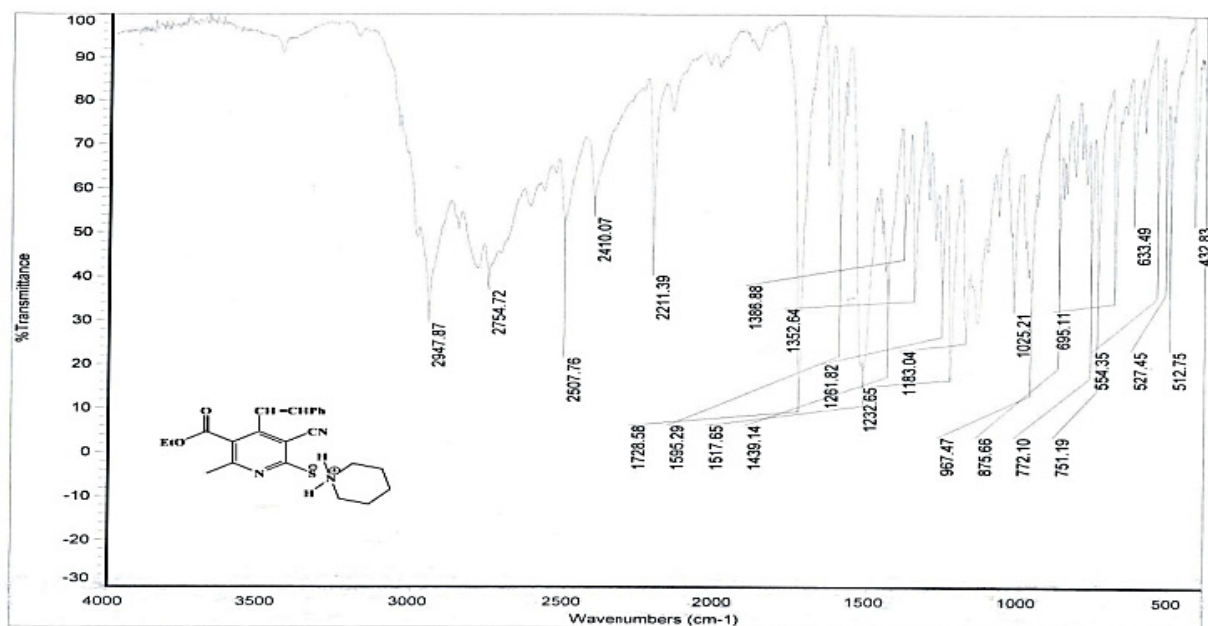


Figure S1. IR spectrum of 4a.

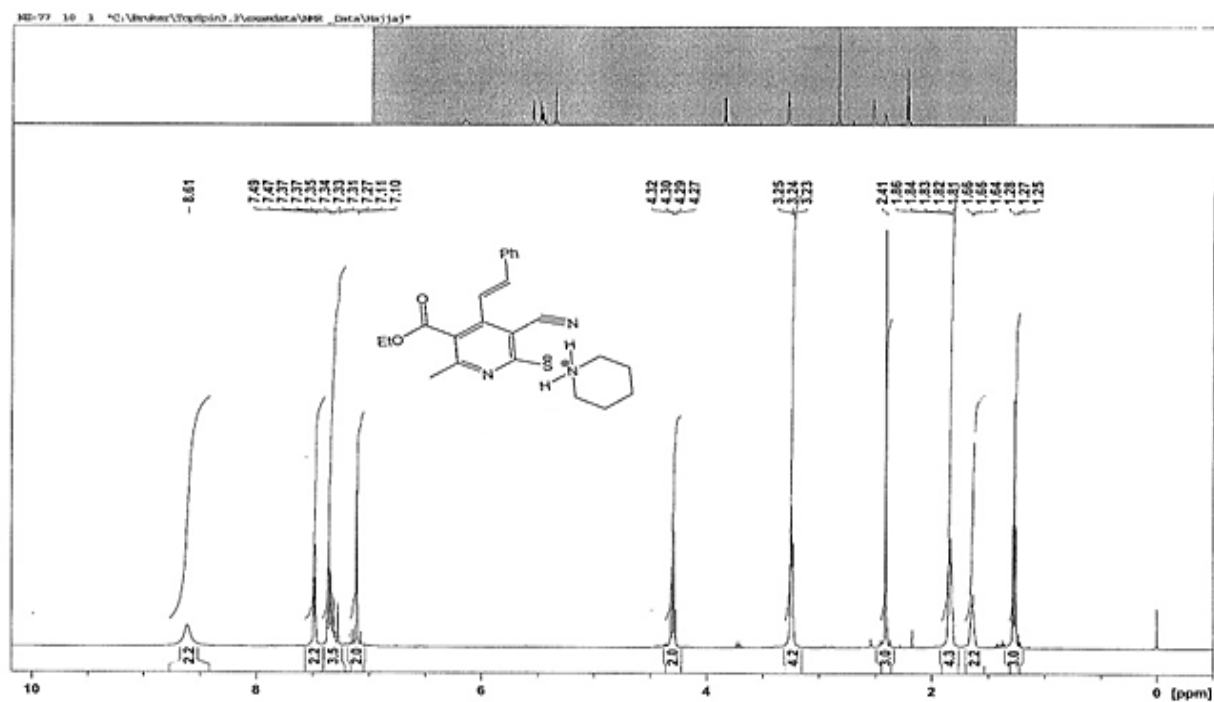


Figure S2. ^1H NMR spectra of 4a.

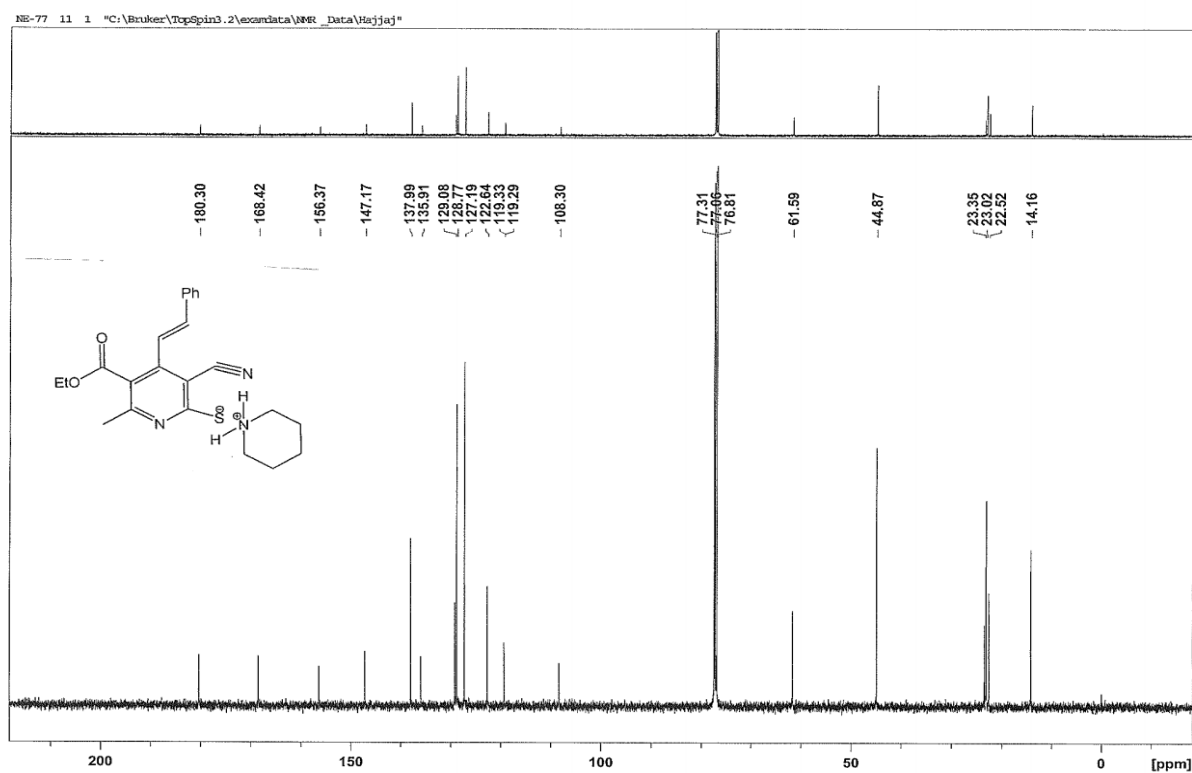


Figure S3. ^{13}C NMR spectra of 4a.

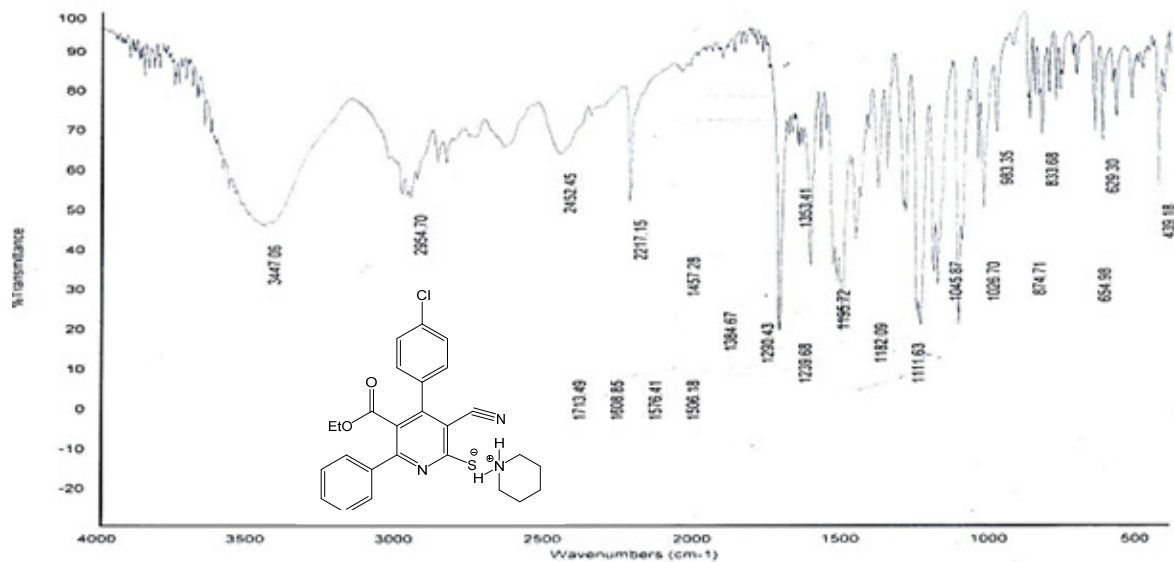


Figure S4. IR spectrum of 4b

SH-8
proton_su CDC13 {C:\nmr-data} Student 23

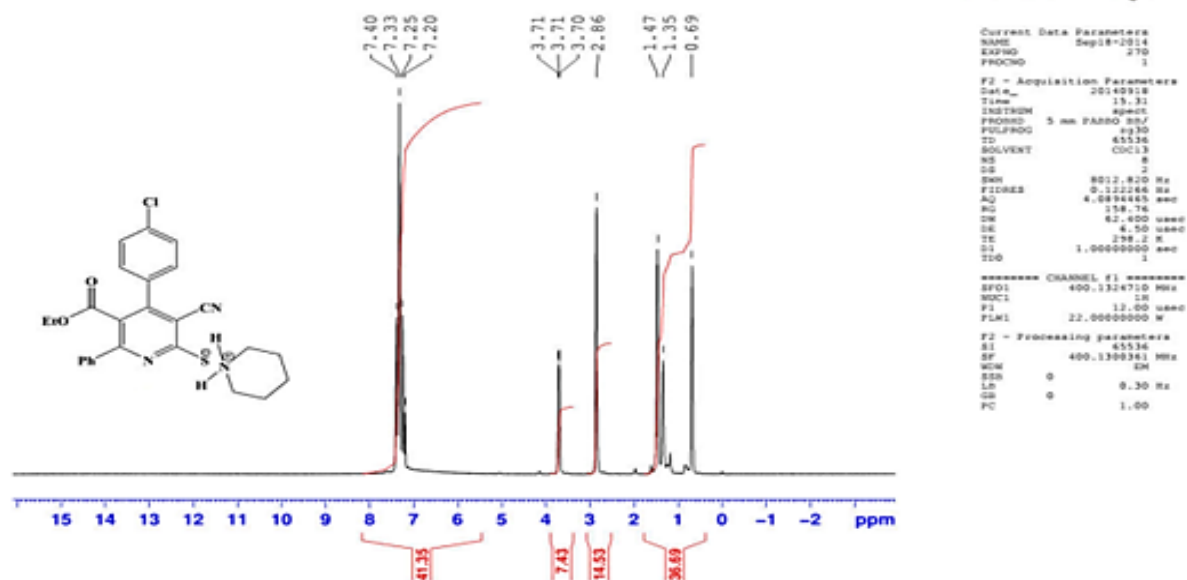


Figure S5. ^1H NMR spectra of 4b.

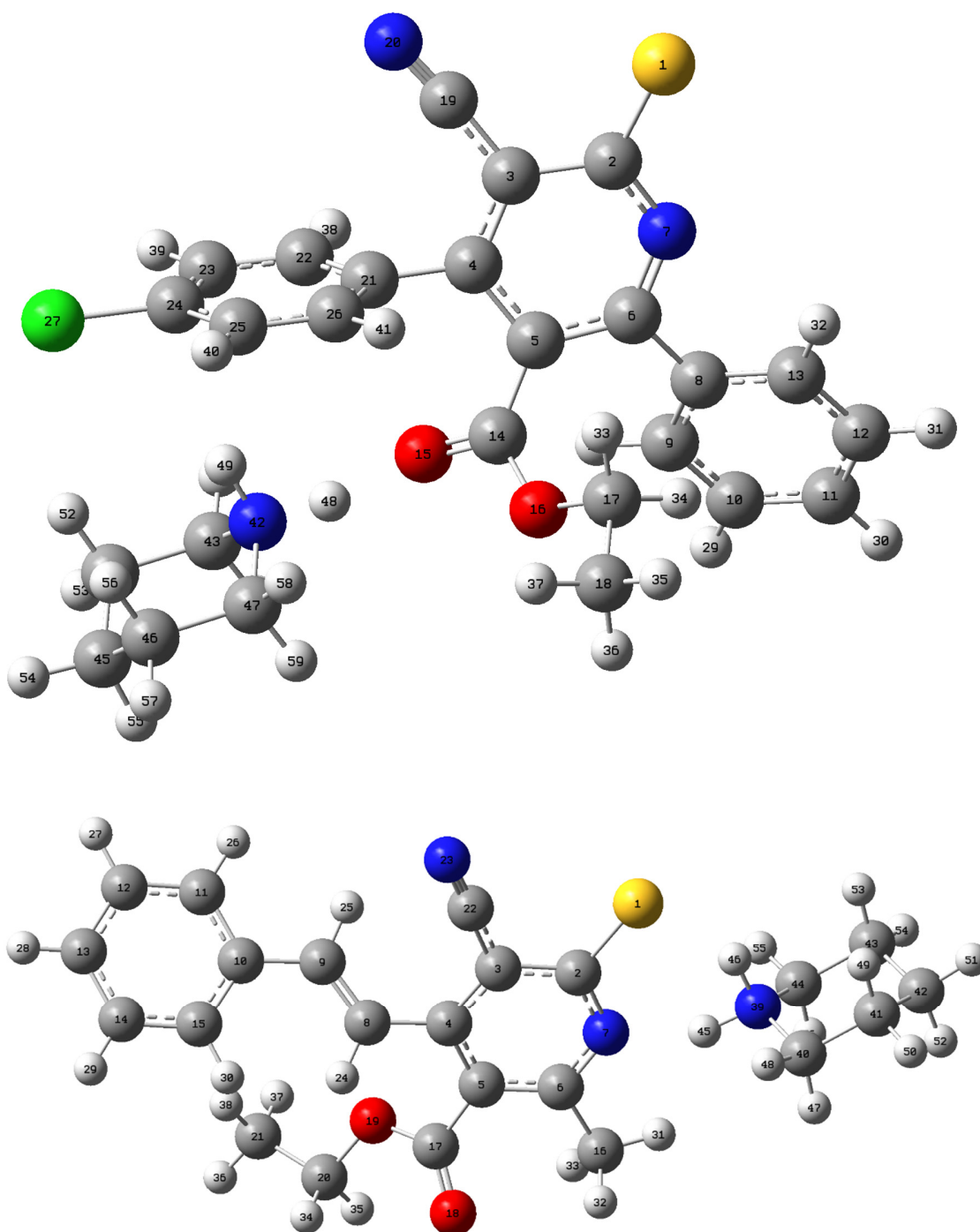


Figure S6. Labeled geometry of compound **4a** and **4b**.

Table S1. Total electronic energy (EE), zero-point correction (ZPE), enthalpy, and free energy of **4a** and **4b**; units are in Hartree

Thermal parameters	4a	4b
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Electronic Energy	-2179.571398	-1605.685199
ZPE	0.472260	0.462140
Enthalpy (ΔH)	-2179.066572	-1605.192886
Free energy (ΔG)	-2179.167935	-1605.288717

Table S2. Optimized coordinated of 4a and 4b at the B3LYP/6-31+G(d,p).

4a				4b			
S	4.09377300	3.72088500	0.39873500	S	2.57059700	-2.27107900	0.16249100
C	3.10527600	2.41889000		C	1.49620000	-0.92672200	-0.01184600
0.00740800				C	0.07866600	-1.12084400	-0.13255000
C	1.65985300	2.54438900	-	C	-0.79887200	-0.02195000	-0.23751600
0.14191000				C	-0.22451100	1.28049800	-0.26245200
C	0.84934500	1.41221600	-	C	1.17710500	1.40877000	-0.18898500
0.14760800				N	1.98492800	0.34906100	-0.05184700
C	1.45587600	0.12333600	-	C	-2.25094100	-0.18389900	-0.41437100
0.08249700				C	-3.03005900	-1.09867000	0.19559900
C	2.88689200	0.08562300	-	C	-4.48016600	-1.25696700	0.03242500
0.22293300				C	-5.14997100	-2.18289700	0.85494500
N	3.63684600	1.16820900	-	C	-6.52806100	-2.37652300	0.75277000
0.18045500				C	-7.26971600	-1.64842000	-0.18019300
C	3.62566600	-1.17344200	-	C	-6.61859300	-0.72914900	-1.01191800
0.54254300				C	-5.24314200	-0.53610100	-0.90872100
C	3.07305100	-2.18157900	-	C	1.87736400	2.74777000	-0.23337700
1.34985600				C	-1.04515300	2.52107000	-0.35241300
C	3.80844300	-3.32834100	-	O	-0.75637700	3.49521000	-1.02953900
1.66012200							
C	5.10701600	-3.48508600	-				
1.17002100							
C	5.67314000	-2.47820300	-				
0.37992100							

C	4.94371400	-1.32984400	-	O	-2.14274800	2.48546700	0.43596900
0.07601800				C	-3.00828800	3.64855500	0.39562300
C	0.60785500	-1.05412700		C	-4.16384300	3.39095200	1.34417900
0.06415000				C	-0.40809300	-2.46565300	-0.20429300
O	-0.42143800	-1.23313500	-	N	-0.82065900	-3.55308600	-0.26901100
0.62027200				H	-2.71274700	0.54617800	-1.07144300
O	0.85832200	-2.00462300		H	-2.57851700	-1.78688200	0.90381000
0.98596100				H	-4.57653600	-2.75821000	1.57687300
C	1.82236800	-1.83370100		H	-7.02017800	-3.09838600	1.39814500
2.06185500				H	-8.34201600	-1.79820400	-0.26561400
C	1.34884800	-2.67084400		H	-7.18610300	-0.16638800	-1.74781200
3.23623700				H	-4.75812900	0.17045100	-1.57510900
C	1.05306700	3.83968500	-	H	2.91714100	2.62582700	0.07893700
0.18565400				H	1.85211000	3.16589500	-1.24389700
N	0.48482600	4.85568500	-	H	1.39902900	3.48527100	0.41583700
0.24797800				H	-3.34442400	3.79900800	-0.63531300
C	-0.63723400	1.58947500	-	H	-2.42403000	4.52723200	0.68545400
0.10536100				H	-4.83936300	4.25297600	1.34048600
C	-1.36932400	1.82713800	-	H	-3.80512000	3.23938500	2.36665000
1.27726600				H	-4.73205900	2.50579900	1.04404300
C	-2.75090000	2.02222800	-	N	4.68363500	-0.08673300	0.06447700
1.23729400				C	5.46139300	0.09364200	-1.19303000
C	-3.40956500	1.97826100	-	C	6.77093500	-0.69504500	-1.13471100
0.00522200				C	7.58274600	-0.33893900	0.12117200
C	-2.70326900	1.76562200		C	6.73582400	-0.52481600	1.39050000
1.18045500				C	5.42701100	0.26280300	1.30666900
C	-1.31869700	1.57407900		H	3.73207900	0.39648200	0.01502600
1.11930900							
Cl	-5.15660200	2.21825500					
0.05557600							
H	2.07936900	-2.06051300	-				
1.76960600							
H	3.36995300	-4.09183500	-				
2.29662500							

H	5.67825200	-4.37690600	-	H	4.27731500	-1.07660000	0.12569600
1.41186900				H	5.65273000	1.16607900	-1.31689400
H	6.68775600	-2.58490000	-	H	4.82100300	-0.23841500	-2.01437200
0.00671300				H	6.54192800	-1.76852500	-1.13857600
H	5.38078700	-0.53084900		H	7.34750100	-0.49043600	-2.04330800
0.51325100				H	8.48399900	-0.95870100	0.17558200
H	1.89027200	-0.77270900		H	7.92163600	0.70480900	0.05566300
2.31654100				H	6.50407000	-1.58842900	1.53143500
H	2.79656800	-2.17026900		H	7.28770900	-0.19987800	2.27918700
1.70227300				H	4.76401100	0.04364600	2.14782900
H	2.07535700	-2.59443200		H	5.61808100	1.34238300	1.29002800
4.05185200							
H	1.25990400	-3.72431700					
2.95472900							
H	0.37930800	-2.32428000					
3.60813200							
H	-0.85195800	1.86741300	-				
2.23033300							
H	-3.30727300	2.22491400	-				
2.14627600							
H	-3.21905400	1.78067800					
2.13497100							
H	-0.76110700	1.43596500					
2.04104800							
N	-2.97196100	-1.48606500	-				
0.20583600							
C	-3.55314600	-1.95431900	-				
1.50936500							
C	-5.07863700	-2.00848200	-				
1.43735600							
C	-5.55393800	-2.86495200	-				
0.25263400							
C	-4.92699600	-2.37575400					
1.06295500							

C 0.96723200	-3.40258600	-2.31611700	
H 0.28599100	-1.90085800	-1.47493200	-
H 0.04920200	-3.23830200	-0.50570300	-
H 1.70057900	-3.12294000	-2.94236300	-
H 2.28127600	-3.19213600	-1.27152400	-
H 1.34468200	-5.47487200	-0.98856900	-
H 2.38429400	-5.45678400	-2.40776300	-
H 0.18134900	-6.64573300	-2.83457800	-
H 0.42313700	-5.27748100	-3.91446300	-
H 1.31306700	-5.31499300	-1.37929100	
H 1.89393400	-5.19729200	-3.03574400	
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H 0.81841600	-2.96871600	-3.30980500	