Supporting Information for

Reductive Benzylation of C₇₀ Imidazoline with a Bulky Addend

Hui-Lei Hou,[†] Zong-Jun Li,[†] Ying Wang,[‡] and Xiang Gao^{*,†}

[†]State Key Laboratory of Electroanalytical Chemistry, [‡]State Key Laboratory of Rare Earth Resources Utilization, Changchun Institute of Applied Chemistry, University of Chinese Academy of Sciences, Chinese Academy of Sciences, 5625 Renmin Street, Changchun, Jilin 130022, China

xgao@ciac.ac.cn

Table of Contents

Figure S1. Cyclic voltammograms of 1 and 1 ²⁻	S4
Figure S2. HPLC trace of the crude product obtained from the reaction of 1 ²⁻ with PhCH ₂ Br	S5
Figure S3. Positive ESI FT-ICR MS of compound 2a	S6
Figure S4. ¹ H NMR spectrum of compound 2a	S7
Figure S5. ¹³ C NMR (DEPTQGPSP) spectrum of compound 2a	S8
Figure S6. HMBC NMR spectrum of 2a	S9
Figure S7. UV-vis spectrum of compound 3a in toluene	S10
Figure S8. Positive ESI FT-ICR MS of compound 3a	S11
Figure S9. ¹ H NMR spectrum of compound 3a	S12
Figure S10. ¹³ C NMR spectrum of compound 3a	S13
Figure S11. HMBC NMR spectrum of 3a	S14
Figure S12. UV-vis spectrum of compound 4a in toluene	S15
Figure S13. Positive ESI FT-ICR MS of compound 4a	S16
Figure S14. ¹ H NMR spectrum of compound 4a	S17

Figure S15. ^{13}C NMR (DEPTQGPSP) spectrum of compound 4a	S18
Figure S16. HMBC NMR spectrum of 4a	S19
Figure S17. HPLC trace of the crude product obtained from the reaction of 1 ²⁻ with <i>o</i> -BrPhCH ₂ Br	S20
Figure S18. UV-vis spectrum of compound 2b in toluene	S21
Figure S19. Positive ESI FT-ICR MS of compound 2b	S22
Figure S20. ^1H NMR spectrum of compound 2b	S23
Figure S21. ^{13}C NMR (DEPTQGPSP) spectrum of compound 2b	S24
Figure S22. UV-vis spectrum of compound 3b in toluene	S25
Figure S23. Positive ESI FT-ICR MS of compound 3b	S26
Figure S24. ^1H NMR spectrum of compound 3b	S27
Figure S25. UV-vis spectrum of compound 4b in toluene	S28
Figure S26. Positive ESI FT-ICR MS of compound 4b	S29
Figure S27. ^1H NMR spectrum of compound 4b	S30
Figure S28. ^{13}C NMR spectrum of compound 4b	S31
Figure S29. UV-vis spectrum of compound 5b in toluene	S32
Figure S30. Positive ESI FT-ICR MS of compound 5b	S33
Figure S31. ^1H NMR spectrum of compound 5b	S34
Figure S32. Calculated LUMOs for 2a and 3a	S35
Figure S33. Cyclic voltammogram of 2b	S36
Cartesian coordinates and the lowest frequencies of 2a , 3a and 2a ²⁻ obtained with Gaussian09	S37
at HF/6-31G level. Total energies of 2a and 3a obtained with Gaussian09 at HF/6-311G(d)	

level

Figure S1. Cyclic voltammograms of (a) **1** and (b) **1**²⁻ in benzonitrile containing 0.1 M TBAP at rt. Scan rate = 0.1 V/s. The arrows indicate the starting potentials and the scan direction for the cyclic voltammetric measurements.

Figure S2. HPLC trace of the crude product obtained from the reaction of **1**²⁻ with PhCH₂Br. The mixture was eluted with a 70:30 v/v mixture of toluene/hexane over a semi-preparative YMC-pack silica column (10 mm × 250 mm) at a flow rate of 3.7 mL/min with the detector wavelength set at 380 nm.

Figure S3. Positive ESI FT-ICR MS of compound **2a**.

Figure S4. ¹H NMR spectrum (500 MHz) of compound **2a** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H₂O residue in DMSO. The resonances at around 0.5 and 1 ppm are due to unknown impurities in the solvent.

Figure S5. ^{13}C NMR (DEPTQGPSP) spectrum (125 MHz) of compound **2a** recorded in CS_2 with $\text{DMSO-}d_6$ as the external lock. The peaks at around 30 and 192 ppm are due to an unknown impurity and CS_2 .

Figure S6. HMBC NMR spectrum of **2a** recorded in CS₂ with DMSO-*d*₆ as the external lock.

Figure S7. UV-vis spectrum of compound **3a** in toluene.

Figure S8. Positive ESI FT-ICR MS of compound **3a**.

Figure S9. ¹H NMR spectrum (500 MHz) of compound **3a** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H₂O residue in DMSO. The resonances between 0.5 and 1 ppm are due to unknown impurities in the solvent.

Figure S10. ^{13}C NMR spectrum (125 MHz) of compound **3a** recorded in CS_2 with $\text{DMSO}-d_6$ as the external lock. The peaks at around 30 and 192 ppm in the NMR correspond to an unknown impurity and CS_2 .

Figure S11. HMBC NMR spectrum of **3a** recorded in CS₂ with DMSO-*d*₆ as the external lock.

Figure S12. UV-vis spectrum of compound **4a** in toluene.

Figure S13. Positive ESI FT-ICR MS of compound **4a**.

Figure S14. ¹H NMR spectrum (500 MHz) of compound **4a** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H₂O residue in DMSO. The resonances at around 0.5 and 1 ppm are due to unknown impurities in the solvent.

Figure S15. ¹³C NMR (DEPTQGPSP) spectrum (125 MHz) of compound **4a** recorded in CS₂ with DMSO-*d*₆ as the external lock. The peaks at around 30 and 192 ppm in the NMR correspond to an unknown impurity and CS₂.

Figure S16. HMBC NMR spectrum of **4a** recorded in CS₂ with DMSO-*d*₆ as the external lock.

Figure S17. HPLC trace of the crude product obtained from the reaction of $\mathbf{1}^{2-}$ with *o*-BrPhCH₂Br. The mixture was eluted with a 70:30 v/v mixture of toluene/hexane over a semi-preparative YMC-pack silica column (10 mm × 250 mm) at a flow rate of 3.7 mL/min with the detector wavelength set at 380 nm. The peak marked with an asterisk is likely due to (*o*-BrPhCH₂)₂C₇₀ according to the retention time.

Figure S18. UV-vis spectrum of compound **2b** in toluene.

Figure S19. Positive ESI FT-ICR MS of compound **2b**.

Figure S20. ¹H NMR spectrum (600 MHz) of compound **2b** recorded in CS₂ with DMSO-*d*₆ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H₂O residue in DMSO. Peak marked with the asterisk is likely due to the toluene residue used for purification of the compound. The resonances at around 0.5 and 1 ppm are due to unknown impurities in the solvent.

Figure S21. ^{13}C NMR spectrum (150 MHz) of compound **2b** recorded in CS_2 with $\text{DMSO}-d_6$ as the external lock. The peaks at around 30 and 192 ppm in the NMR correspond to an unknown impurity and CS_2 .

Figure S22. UV-vis spectrum of compound **3b** in toluene.

Figure S23. Positive ESI FT-ICR MS of compound **3b**.

Figure S24. ¹H NMR spectrum (600 MHz) of compound **3b** recorded in CS₂ with CD₃COCD₃ as the external lock. The resonance at around 2.05 ppm is due to the acetone solvent, and the resonances at around 2.78 and 2.81 ppm are due to the H₂O and unidentified impurity residue in CD₃COCD₃. The resonances between 0 and 0.7 ppm are due to unknown impurities in the solvent.

Figure S25. UV-vis spectrum of compound **4b** in toluene.

Figure S26. Positive ESI FT-ICR MS of compound **4b**.

Figure S27. ^1H NMR spectrum (600 MHz) of compound **4b** recorded in CS_2 with $\text{DMSO}-d_6$ as the external lock. The resonance at around 2.5 ppm is due to the DMSO solvent, and the resonance at around 3.3 ppm is due to the H_2O residue in DMSO. Peaks marked with asterisks are due to the toluene residue used for purification of the compound. The resonances at around 0.5 and 1 ppm are due to unknown impurities in the solvent.

Figure S28. ^{13}C NMR spectrum (150 MHz) of compound **4b** recorded in CS_2 with $\text{DMSO}-d_6$ as the external lock. The peaks at around 30 and 192 ppm in the NMR correspond to an unknown impurity and CS_2 . The resonance at around 109 ppm is due to an artifact from the instrument.

Figure S29. UV-vis spectrum of compound **5b** in toluene.

Figure S30. Positive ESI FT-ICR MS of compound **5b**.

Figure S31. ^1H NMR spectrum (600 MHz) of compound **5b** recorded in CS_2 with CD_3COCD_3 as the external lock. The resonance at around 2.05 ppm is due to the acetone solvent, and the resonances at around 2.78 and 2.81 ppm are due to the H_2O and unidentified impurity residue in CD_3COCD_3 . The resonances between 0 and 1 ppm are due to unknown impurities in the solvent.

Figure S32. Calculated LUMOs for (a) **2a** and (b) **3a**

Figure S33. Cyclic voltammogram of **2b** (1,2,3,16-adduct) in benzonitrile containing 0.1 M TBAP at rt. Scan rate = 0.1 V/s. The arrows indicate the starting potentials (0 V vs SCE) and the scan direction for the cyclic voltammetric measurements.

Cartesian coordinates and the lowest frequencies of **2a**, **3a** and **2a²⁻** obtained with Gaussian09 at HF/6-31G level. Total energies of **2a** and **3a** obtained with Gaussian09 at HF/6-311G(d) level.

Geometry of **2a**

Charge = 0 Multiplicity = 1

C	1.38130200	2.54475000	0.33313300
C	2.16323600	1.54028100	-0.66230500
C	2.42238100	0.01325000	-0.15530100
C	1.64584500	-0.39914300	1.06387600
C	0.92974400	0.57352500	1.89418200
C	0.69958600	1.83356700	1.49747600
C	-3.02877900	-3.50851200	-0.80272000
C	-2.68953400	-3.46057200	0.58123500
C	-4.56628700	-1.02379000	2.57682600
C	-3.68009100	-2.14994400	2.38325800
C	-3.85054600	-2.97476700	1.30975500
C	-4.91508700	-2.72612000	0.36530100
C	-4.39844000	-3.04113400	-0.94660800
C	-5.58145300	-0.77609700	1.67856500
C	-5.76322600	-1.65402000	0.53923700
C	-4.74491200	-2.27332900	-2.02118700
C	-5.63088500	-1.14462500	-1.84886800
C	-5.84009600	0.58328500	1.24339600
C	-6.17755300	0.54345600	-0.16843300
C	-6.13147200	-0.83861100	-0.60168400
C	-1.58371500	3.18278200	-2.01683200
C	-1.75763400	2.32762400	-3.12730900
C	-0.48098900	1.69263800	-3.41016100
C	-0.44173900	0.39850300	-3.85188600
C	0.56333500	-0.47886200	-3.33969600
C	1.48584800	-0.01598200	-2.40681800
C	1.89627700	-0.84841000	-1.31781900
C	0.12967200	3.17568600	-0.29262800
C	0.49768000	2.17575100	-2.48224100
C	-0.19192200	3.12340800	-1.59467200
C	1.45564600	1.34375900	-1.99189700
C	-0.58482100	2.44887400	1.78387300
C	-0.93543000	3.25100600	0.68449200
C	1.03929100	-1.59577800	1.21820100
C	-0.04716800	-1.48100300	2.19386800
C	-0.10156900	-0.14886600	2.61653700
C	-1.30828600	0.45506700	3.02728400
C	-1.56432200	1.82425800	2.58134900

C	-2.89251000	2.23192700	2.37568200
C	-3.24789100	3.02807700	1.25639900
C	-2.28802500	3.44773000	0.32256600
C	-2.62839900	3.41315500	-1.10221600
C	-3.90183500	2.95225100	-1.48132200
C	-4.07602600	2.09262000	-2.59568000
C	-2.97925600	1.66349000	-3.36515000
C	-2.93877800	0.25952700	-3.81642000
C	-1.67884900	-0.35124000	-4.00016000
C	-1.43367700	-1.67537400	-3.57313100
C	-0.03948400	-1.76029300	-3.15827900
C	0.30874300	-2.50743000	-2.06740500
C	1.31638100	-2.06989900	-1.15239700
C	-0.38246200	-3.22111500	0.01816700
C	-1.38491300	-3.19161500	1.00840600
C	-1.20268200	-2.28702900	2.16764200
C	-2.33929000	-1.76449300	2.79511800
C	-2.39248200	-0.40447300	3.22397100
C	-3.76105100	0.06421600	3.08200700
C	-4.00464600	1.34554100	2.67365100
C	-5.06836500	1.61318700	1.73063100
C	-4.59183400	2.65016200	0.84157700
C	-4.90692500	2.61212500	-0.48500400
C	-5.72091100	1.53592300	-1.00671700
C	-5.19392500	1.20518400	-2.31047800
C	-5.15076500	-0.09688000	-2.71901000
C	-3.99013500	-0.59347800	-3.44391100
C	-3.74345900	-1.92652300	-3.01574300
C	-2.43734500	-2.44079200	-2.94714000
C	-2.06713600	-3.25818100	-1.78056800
C	-0.71854600	-3.23166900	-1.33139800
C	4.40344100	1.22597600	-0.56293500
C	5.83963800	1.57730400	-0.56913400
C	6.35019000	2.31571200	-1.63192000
H	5.70439300	2.57785800	-2.44566800
C	7.67693300	2.71330400	-1.62877000
H	8.06613100	3.27580300	-2.45479300
C	8.49802400	2.39049800	-0.55715100
H	9.52460700	2.70184900	-0.55380600
C	7.98729500	1.67177100	0.51359100
H	8.61372800	1.43291300	1.35062600
C	6.66265400	1.26363800	0.50848200
H	6.27410200	0.72444100	1.35088000
C	4.64617400	-1.13598900	0.25354100

C	5.64948000	-1.66079000	-0.70656600
C	5.57470000	-1.39718900	-2.07063200
H	4.80126700	-0.76555100	-2.45901900
C	6.48812200	-1.97103000	-2.94077400
H	6.42029700	-1.77190000	-3.99213300
C	7.48461900	-2.80256000	-2.45106700
H	8.19436200	-3.24165800	-3.12522600
C	7.56159600	-3.07231000	-1.09052500
H	8.32901000	-3.71851500	-0.71204800
C	6.64254700	-2.50983600	-0.22267800
H	6.68110300	-2.72273800	0.82673500
N	3.91109600	0.01226400	-0.07766300
N	3.51275100	2.06056200	-0.91462500
O	4.41255800	-1.72869300	1.29463300
C	2.37742300	3.64474100	0.85950700
H	3.19701100	3.13093000	1.34274600
H	2.79124400	4.14003200	-0.00420700
C	1.80945700	4.67192000	1.81534600
C	1.27513600	5.86651000	1.33854900
C	1.85608800	4.47137300	3.19269500
C	0.78219300	6.82546100	2.21127100
H	1.24643000	6.04853800	0.28048300
C	1.36463900	5.42754200	4.06956300
H	2.27967800	3.56440300	3.58212600
C	0.82290900	6.60727100	3.58074100
H	0.37347600	7.73908600	1.82398400
H	1.40830000	5.25321500	5.12758800
H	0.44358300	7.34861300	4.25737400
C	1.06077200	-2.72003000	0.21499100
C	2.03952300	-3.90190600	0.52387500
H	1.94019300	-4.61326900	-0.28821200
H	3.04517100	-3.51435600	0.49723400
C	1.80762600	-4.59789300	1.84746600
C	2.41640700	-4.12295800	3.00800900
C	1.00533600	-5.73276500	1.93052400
C	2.21371300	-4.76117900	4.22271800
H	3.05176800	-3.25992900	2.95307300
C	0.80247900	-6.37308900	3.14494300
H	0.53933000	-6.12008800	1.04369700
C	1.40479800	-5.88663200	4.29552400
H	2.68887300	-4.38307000	5.10772400
H	0.18075700	-7.24678900	3.19020700
H	1.24984900	-6.38046200	5.23568000

Lowest frequency = 19.22 cm⁻¹

Total energy = -3909.2750 hartree (1 hartree = 627.51 kcal/mol)

Geometry of **3a**

Charge = 0 Multiplicity = 1

C	1.46764700	1.65757900	-1.35867900
C	2.19318400	0.22522900	-1.25673600
C	2.36026300	-0.47557700	0.22030100
C	1.82921800	0.32769200	1.50142000
C	0.87678100	1.45944200	1.12039200
C	0.73405500	2.02899600	-0.07862400
C	-3.35684500	-3.07552600	2.09689400
C	-3.03214200	-2.05314900	3.02299100
C	-4.73242400	1.15126500	2.47497100
C	-3.93087100	0.20654900	3.22304700
C	-4.15781200	-1.13285100	3.09403900
C	-5.19505700	-1.60972400	2.20728700
C	-4.68965900	-2.80693700	1.57620400
C	-5.72288500	0.70588500	1.62872300
C	-5.96274700	-0.71793200	1.49016100
C	-4.97387000	-3.05993400	0.26520200
C	-5.78020000	-2.13349800	-0.49393600
C	-5.88056700	1.31545900	0.32062300
C	-6.21648200	0.26743600	-0.62432100
C	-6.26530200	-0.98713600	0.09885300
C	-1.44201400	0.49126500	-3.58135100
C	-1.67120800	-0.89797000	-3.71269000
C	-0.44058000	-1.58967800	-3.37224800
C	-0.49217100	-2.78998400	-2.71552400
C	0.44508600	-3.04845400	-1.67112300
C	1.38401100	-2.07542500	-1.33262900
C	1.69142500	-1.82848200	0.03080100
C	0.26010400	1.67235400	-2.31307200
C	0.56930100	-0.61976800	-3.05205200
C	-0.05725200	0.70152800	-3.18642300
C	1.47328500	-0.85760100	-2.06148500
C	-0.51124200	2.69984400	-0.40264400
C	-0.80024900	2.48092200	-1.76117700
C	0.83878200	-0.49662300	2.36151800
C	-0.24037300	0.34717700	2.82637500
C	-0.20944600	1.53846500	2.07946200
C	-1.36841200	2.29817500	1.85244200
C	-1.52823300	2.91218100	0.53975900
C	-2.82402600	3.11241300	0.03254800

C	-3.12380700	2.86109000	-1.32742800
C	-2.13275600	2.41437900	-2.21979900
C	-2.47220900	1.36383300	-3.18177800
C	-3.77411000	0.82882000	-3.16232900
C	-4.00285900	-0.56343100	-3.29628600
C	-2.93477500	-1.46656300	-3.44623500
C	-2.98918100	-2.74932200	-2.71801000
C	-1.77771800	-3.35357400	-2.33200300
C	-1.62501200	-3.94816200	-1.05453800
C	-0.24561900	-3.75438100	-0.63925200
C	0.03500900	-3.47126600	0.66987400
C	1.03759600	-2.50603100	1.00621900
C	0.58942100	-1.81106600	2.21735700
C	-0.70487300	-2.37268100	2.57300300
C	-1.70771400	-1.60194000	3.18732400
C	-1.46352700	-0.16393800	3.31766600
C	-2.56639200	0.70898900	3.28851100
C	-2.51697300	1.92850500	2.57336900
C	-3.84729900	2.21612900	2.05998500
C	-3.99647800	2.79007000	0.82963200
C	-5.03873200	2.33474600	-0.06282300
C	-4.48814300	2.36226800	-1.40100500
C	-4.80422900	1.37645300	-2.29054700
C	-5.68700600	0.30242100	-1.89644200
C	-5.17909000	-0.90409400	-2.50804300
C	-5.22478200	-2.08551400	-1.82619800
C	-4.09763800	-3.00436600	-1.88980600
C	-3.94423700	-3.60002200	-0.61119800
C	-2.67723700	-3.96016500	-0.11830200
C	-2.36752000	-3.67655900	1.29760300
C	-1.03236300	-3.39386000	1.64824900
C	4.41256500	-0.12168600	-0.91998500
C	5.86799100	0.06763300	-1.08980100
C	6.39885600	0.12798000	-2.37493200
H	5.75092400	-0.01744900	-3.21560300
C	7.74752500	0.38048000	-2.55935400
H	8.15134800	0.41836000	-3.55217100
C	8.57380500	0.58837200	-1.46295600
H	9.61822500	0.78652400	-1.60698600
C	8.04577800	0.54524800	-0.18131600
H	8.67732000	0.71685100	0.66828600
C	6.69753800	0.28324400	0.00617400
H	6.29671700	0.26574700	1.00081400
C	4.38433800	-1.79039300	0.95027400

C	5.36388200	-2.72345000	0.33455600
C	5.27244400	-3.11934500	-0.99553600
H	4.51611900	-2.71013400	-1.63564300
C	6.14354900	-4.07324500	-1.49768200
H	6.06093500	-4.38341100	-2.52074500
C	7.11526600	-4.62665700	-0.67709000
H	7.79329400	-5.35973200	-1.06929300
C	7.20429600	-4.24063800	0.65386800
H	7.94873400	-4.67449600	1.29214400
C	6.32272300	-3.30205100	1.16099100
H	6.36364000	-3.01777500	2.19333900
N	3.84312100	-0.73767900	0.20905800
N	3.57523100	0.36851000	-1.73474300
O	3.99650900	-1.98692800	2.09408500
C	3.03786100	0.90554100	2.32158600
H	3.65980500	0.07797900	2.60839700
H	3.60519800	1.53071400	1.64183600
C	2.51328700	2.76060300	-1.76996700
H	3.30630500	2.74692800	-1.03489000
H	2.95744600	2.45113400	-2.70217300
C	2.69795900	1.70424000	3.56215000
C	2.56368500	1.06148900	4.79132100
C	2.56512100	3.08899400	3.52115700
C	2.28343600	1.78092800	5.94320700
H	2.68149100	-0.00464600	4.84429300
C	2.28611600	3.81327100	4.67145600
H	2.68155800	3.60517100	2.58676100
C	2.14101900	3.16022100	5.88620900
H	2.18152800	1.26799100	6.88031000
H	2.18595700	4.88055900	4.61902000
H	1.92579000	3.71826900	6.77705300
C	1.99047300	4.17538800	-1.90415000
C	1.53332700	4.64833500	-3.13222200
C	2.00752100	5.05406500	-0.82444700
C	1.08602900	5.95355000	-3.27266900
H	1.52804800	3.99264700	-3.98276200
C	1.56137200	6.36081700	-0.95912800
H	2.37386900	4.71642400	0.12678600
C	1.09576800	6.81409600	-2.18437500
H	0.73627500	6.29742900	-4.22719700
H	1.58140700	7.02137600	-0.11348400
H	0.75147300	7.82466800	-2.29141300

Lowest frequency = 22.32 cm⁻¹

Total energy = -3909.2718 hartree (1 hartree = 627.51 kcal/mol)

Geometry of **2a²⁻**

Charge = -2 Multiplicity = 1

C	1.35236700	2.53812100	0.38858400
C	2.13468900	1.51918000	-0.58091400
C	2.37289000	-0.00392800	-0.05364100
C	1.60976300	-0.40053000	1.16889600
C	0.91641900	0.54331500	1.98462300
C	0.66363500	1.86227700	1.57898100
C	-3.06272000	-3.50197900	-0.78064400
C	-2.74588900	-3.45642100	0.61121400
C	-4.58244300	-0.96790400	2.56494600
C	-3.72042600	-2.11893600	2.38860700
C	-3.90843900	-2.95444600	1.31794900
C	-4.94887800	-2.68254000	0.35716300
C	-4.42431900	-3.01506900	-0.94697600
C	-5.58142700	-0.70525300	1.64621200
C	-5.76890100	-1.57990000	0.51165400
C	-4.73974900	-2.24793400	-2.03454200
C	-5.61016100	-1.10032200	-1.89093500
C	-5.79836300	0.65937900	1.19164800
C	-6.13445900	0.61145100	-0.22992900
C	-6.11355600	-0.76717600	-0.64119500
C	-1.51164500	3.20740200	-2.04983900
C	-1.69100700	2.33212800	-3.19993800
C	-0.45068800	1.66937000	-3.40294700
C	-0.38767900	0.35531300	-3.83893500
C	0.58785600	-0.51467000	-3.28372100
C	1.48636400	-0.04570400	-2.32205600
C	1.86550100	-0.86883700	-1.21855500
C	0.11908700	3.20054200	-0.26034800
C	0.51150700	2.16150800	-2.44272700
C	-0.16776600	3.16080900	-1.62394800
C	1.44632300	1.31627100	-1.92129100
C	-0.54425700	2.46448200	1.83418600
C	-0.89913800	3.30387900	0.66650700
C	0.99190300	-1.63763800	1.32449500
C	-0.06192100	-1.52160000	2.26303400
C	-0.11455300	-0.15156400	2.67073800
C	-1.33744400	0.46781000	3.04366800
C	-1.57503500	1.82687500	2.59506900
C	-2.89157900	2.25975600	2.39462200
C	-3.24913200	3.09906000	1.21972700

C	-2.25684500	3.46598300	0.28013100
C	-2.57603600	3.43083000	-1.13431100
C	-3.86034100	2.97964500	-1.52799600
C	-4.04248100	2.12126000	-2.69032000
C	-2.91797300	1.66018200	-3.40390600
C	-2.88334500	0.24708200	-3.82915700
C	-1.62335300	-0.38226800	-3.98316300
C	-1.39942800	-1.71596600	-3.54864800
C	-0.02348900	-1.79786600	-3.09844000
C	0.30407000	-2.53529400	-1.99178400
C	1.29384400	-2.09801800	-1.06046300
C	-0.42335600	-3.24683600	0.08566200
C	-1.44202000	-3.20171200	1.06178900
C	-1.25871000	-2.29958900	2.22122100
C	-2.38872800	-1.77861600	2.83842600
C	-2.44107300	-0.38048000	3.25353800
C	-3.76821100	0.09686800	3.09771900
C	-3.98173300	1.40841400	2.66130300
C	-5.02254200	1.67737800	1.68208500
C	-4.52754700	2.72492800	0.79753900
C	-4.86282200	2.68932500	-0.56957600
C	-5.65742500	1.59897600	-1.07192300
C	-5.12517700	1.24191700	-2.37630000
C	-5.11849800	-0.08134500	-2.77235600
C	-3.94960200	-0.59445300	-3.45823600
C	-3.72624900	-1.93876700	-3.02674600
C	-2.42508800	-2.45683700	-2.92518000
C	-2.08135900	-3.26928500	-1.74413100
C	-0.73911000	-3.25395300	-1.27086100
C	4.37895100	1.18268500	-0.50594400
C	5.82006700	1.52899900	-0.53602000
C	6.31477300	2.28136400	-1.59703700
H	5.64843300	2.55689200	-2.38940800
C	7.64242400	2.67590900	-1.61612200
H	8.01460100	3.25103500	-2.44258200
C	8.48708900	2.33466900	-0.56835900
H	9.51567600	2.64285800	-0.58223400
C	7.99458800	1.60094900	0.50009600
H	8.63687300	1.34541800	1.32123800
C	6.66730600	1.19806200	0.51700900
H	6.29081900	0.64673200	1.35666800
C	4.63455700	-1.17344200	0.24158700
C	5.56791400	-1.66943800	-0.81661800
C	5.36242800	-1.39409900	-2.16356800

H	4.53480400	-0.78573700	-2.46786000
C	6.20911000	-1.93387100	-3.12139900
H	6.03532700	-1.72682800	-4.15953100
C	7.26766700	-2.74250900	-2.73773100
H	7.92387300	-3.15613500	-3.48039500
C	7.47358100	-3.02529300	-1.39311300
H	8.28781000	-3.65725300	-1.09346100
C	6.62138700	-2.49766000	-0.43883200
H	6.75395700	-2.72399300	0.60013300
N	3.89402200	-0.02302700	-0.00294900
N	3.49880000	2.02733900	-0.84313500
O	4.51172800	-1.81342900	1.27505800
C	2.36877500	3.63085800	0.89498600
H	3.17901000	3.11204800	1.39139500
H	2.79629700	4.10438800	0.02492600
C	1.84816300	4.70172400	1.82940900
C	1.37690700	5.91385600	1.33061500
C	1.89741900	4.53689500	3.21177900
C	0.96389100	6.92792400	2.18257700
H	1.32124700	6.05600100	0.26811800
C	1.48692300	5.54739700	4.06875900
H	2.24494400	3.60524800	3.61552800
C	1.01863100	6.74884200	3.55693600
H	0.59404000	7.84975900	1.77326100
H	1.52424100	5.39206100	5.13101600
H	0.69386700	7.53027300	4.21897500
C	1.02038000	-2.74869100	0.30475800
C	1.99872700	-3.93694500	0.58120900
H	1.90261200	-4.63247000	-0.24690100
H	3.00381500	-3.54477200	0.56200100
C	1.78985600	-4.67535100	1.88386200
C	2.36716300	-4.20386800	3.06274200
C	1.04151500	-5.84827100	1.93634700
C	2.19740800	-4.88810300	4.25673400
H	2.93889200	-3.29696600	3.03477800
C	0.87020100	-6.53533500	3.13050800
H	0.58194600	-6.21928300	1.03928300
C	1.44945400	-6.05723900	4.29589900
H	2.64180400	-4.50391700	5.15601100
H	0.28148300	-7.43392600	3.14933300
H	1.31390500	-6.58280500	5.22325200

Lowest frequency = 19.52 cm^{-1}