Supporting Information for

Preparation and Characterisation of an Equatorial Para-adduct of $(PhCH_2)HC_{70}$ from the Reaction of C_{70}^{2-} with Benzyl Bromide and H_2O: Addition Effects in the Polar and Equatorial Regions of C_{70}

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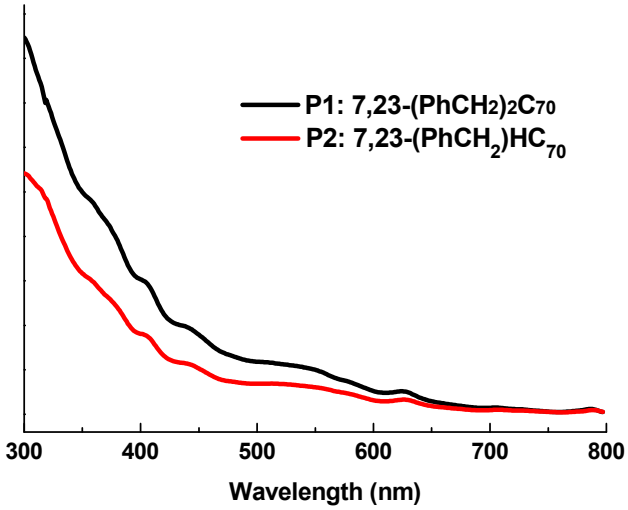

Figure S1. UV-vis absorption spectra of 7,23-$(PhCH_2)HC_{70}$ and 7,23-$(PhCH_2)_2C_{70}$ recorded in toluene.

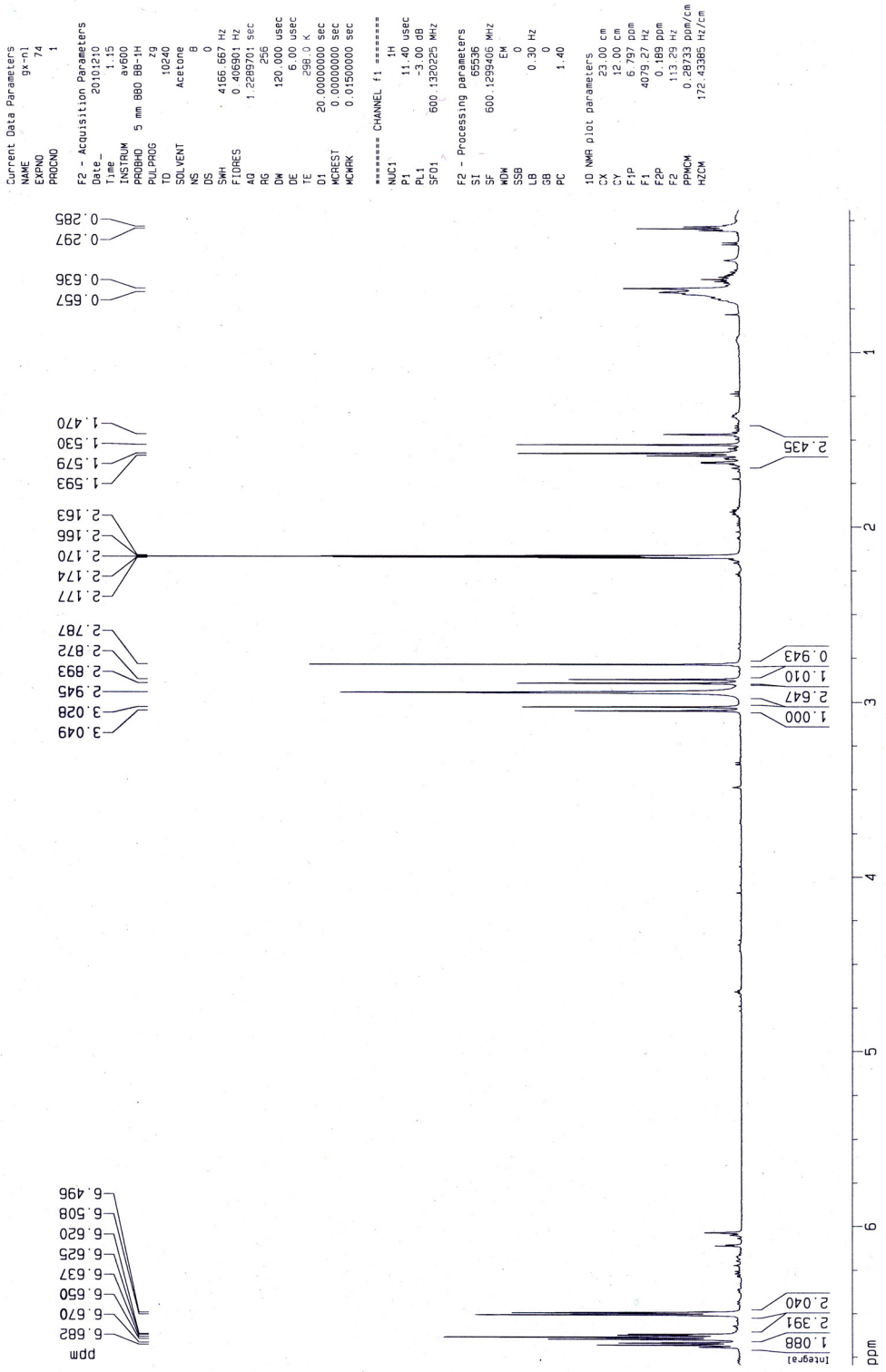

Figure S2. ^{1}H NMR spectrum of 7,23-($PhCH_2$)HC_{70} recorded in CS_2 with acetone-d_6 as the external lock.

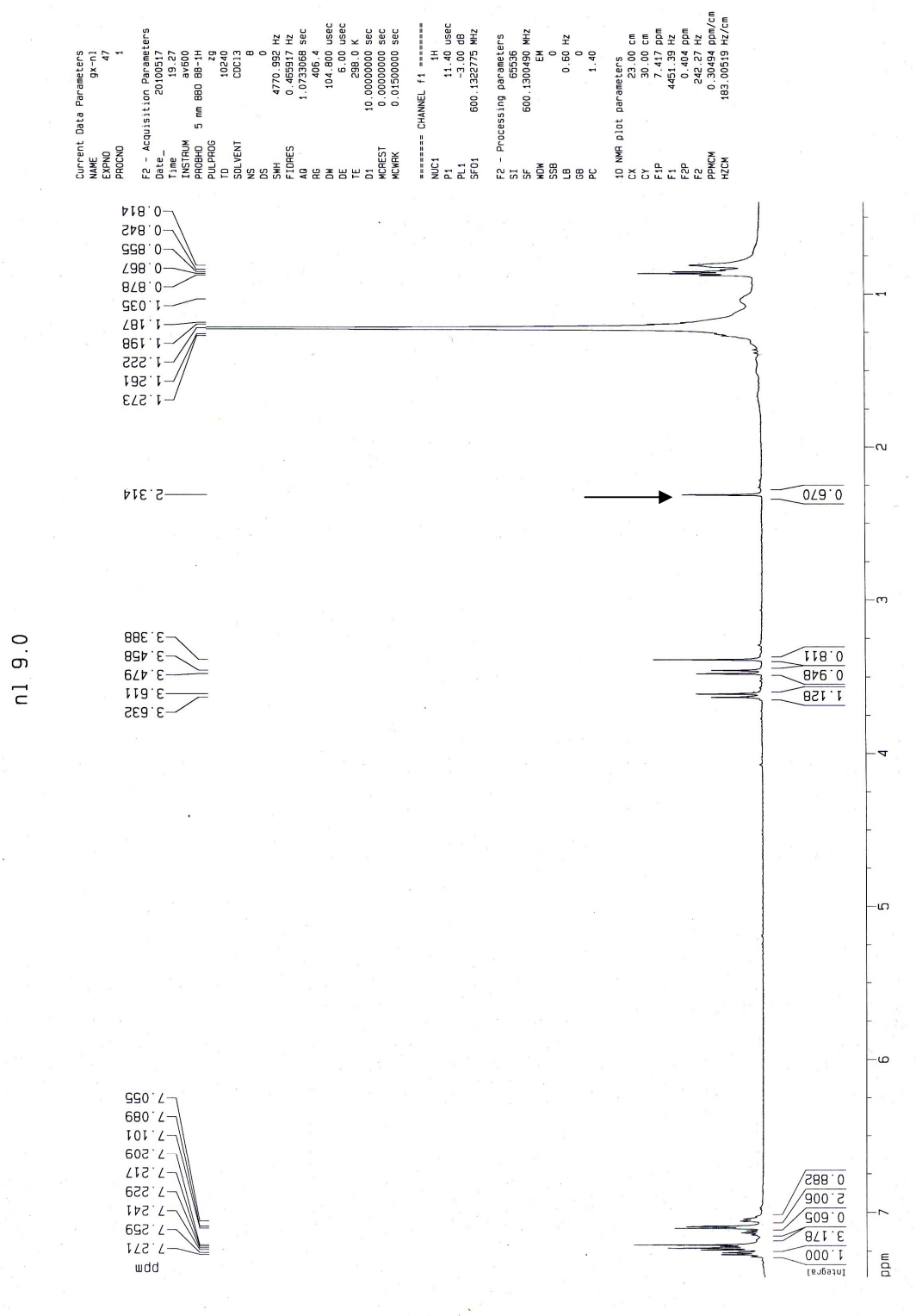

Figure S3. ^{1}H NMR spectrum of 7,23-(PhCH$_2$)HC$_{70}$ recorded in CS$_2$/CDCl$_3$. The peak labeled with an arrow is from the toluene residue used for HPLC purification.

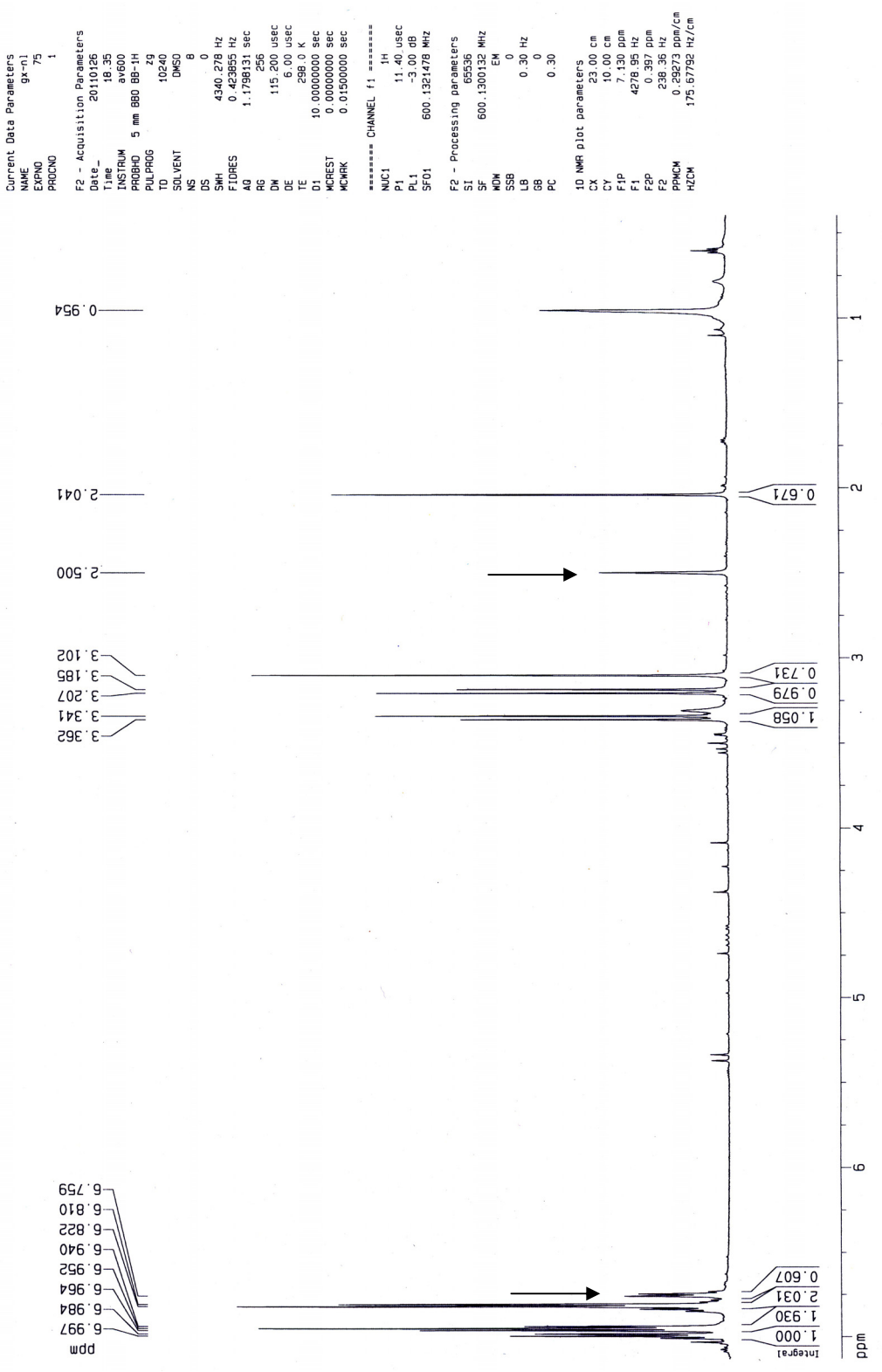

Figure S4. ^{1}H NMR spectrum of 7,23-(PhCH$_2$)HC$_{70}$ recorded in CS$_2$ with DMSO-d_6 as the external lock. Peaks labeled with arrows are from the toluene residue used for HPLC purification.

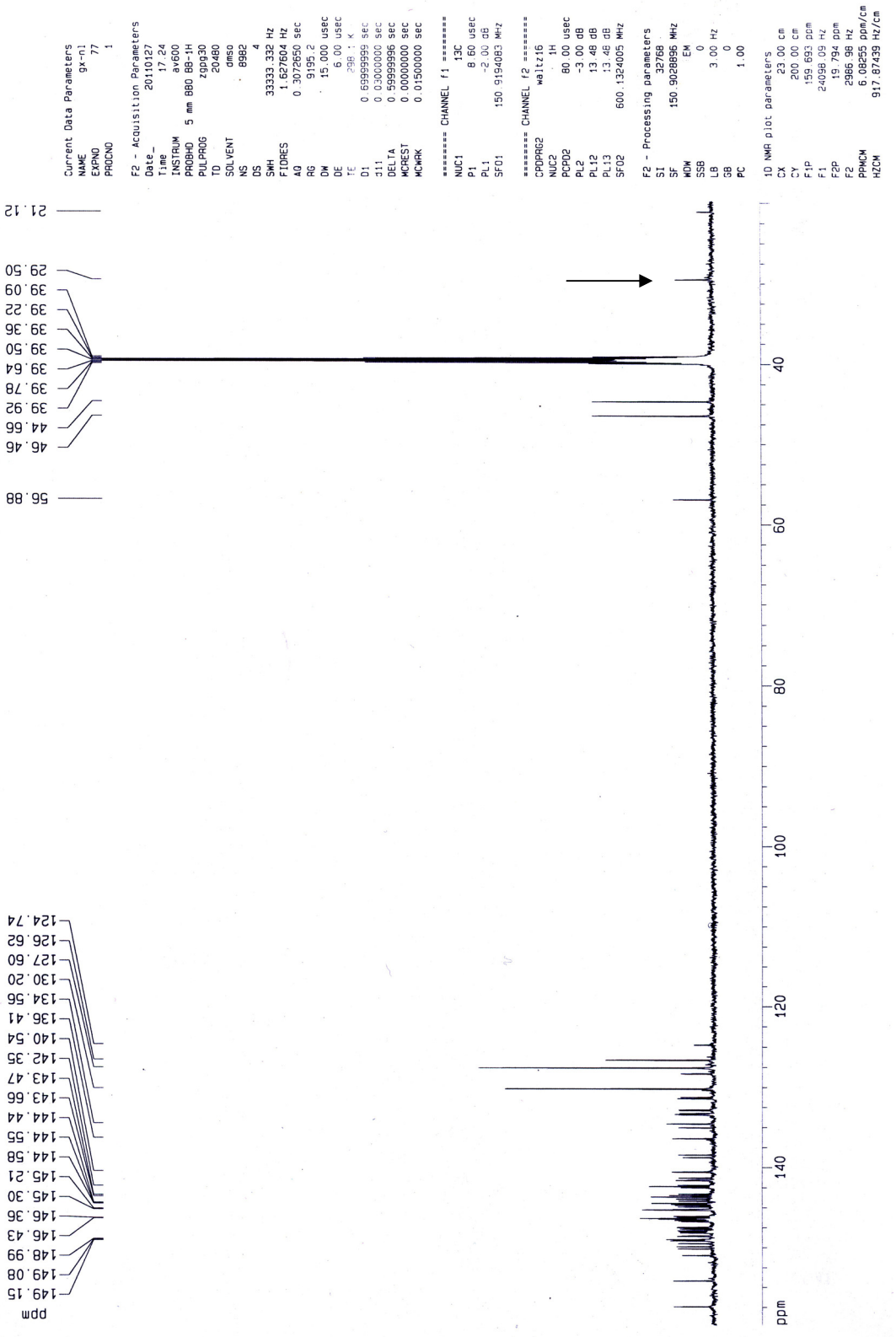

Figure S5. ^{13}C NMR spectrum of 7,23-($PhCH_2$)HC_{70} in CS_2 with DMSO-d_6 as the external lock. The peak labeled with an arrow is from the toluene residue used for HPLC purification.

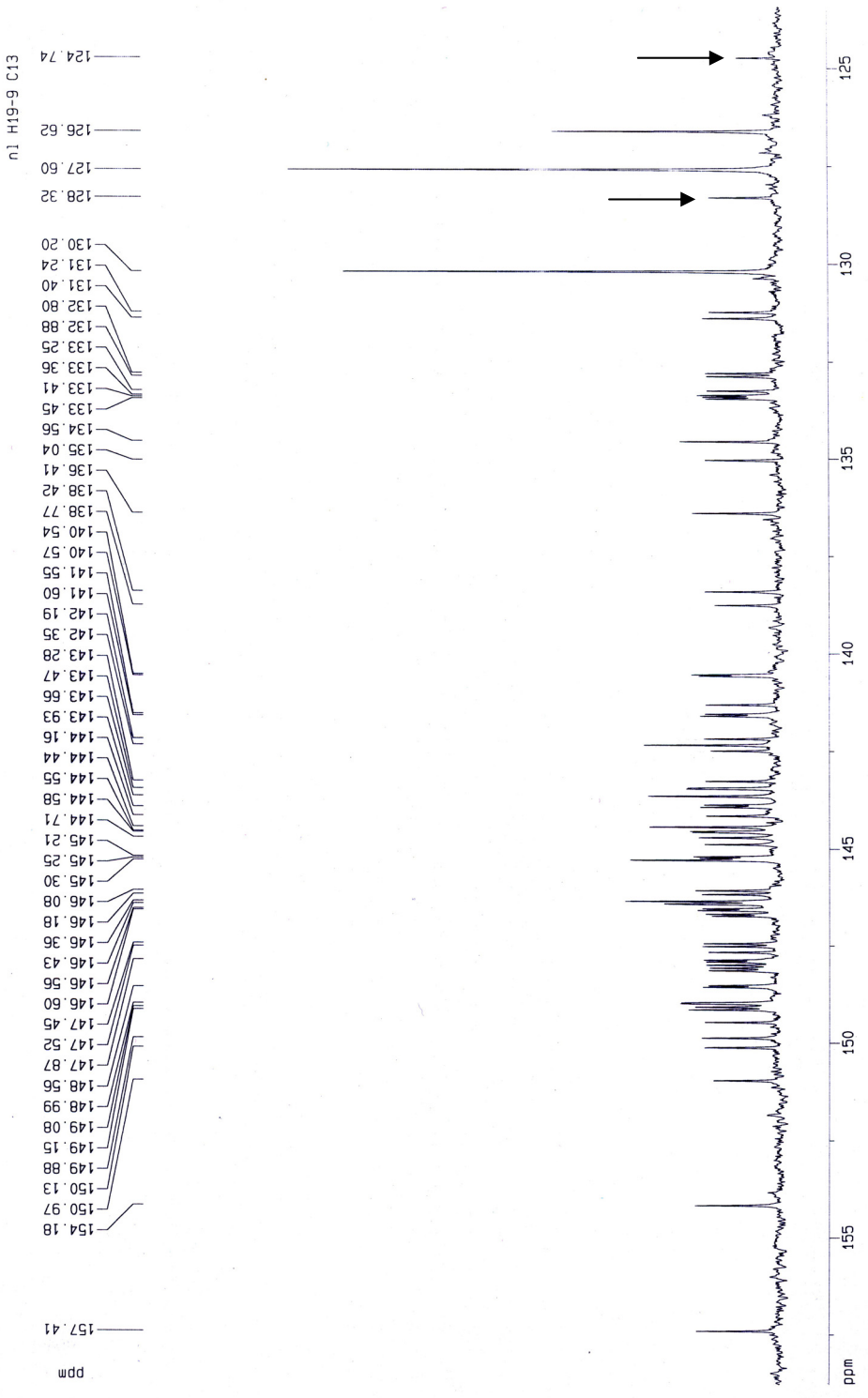

Figure S6. Expanded ^{13}C NMR spectrum for the sp^2 region of 7,23-$(PhCH_2)HC_{70}$ in CS_2 with DMSO-d_6 as the external lock. Peaks labeled with arrows are due to the toluene residue used for HPLC purification. One of the toluene resonances is coincidentally overlapped with a phenyl carbon atom of the addend at 127.60 ppm, and the last one is too weak to assign.

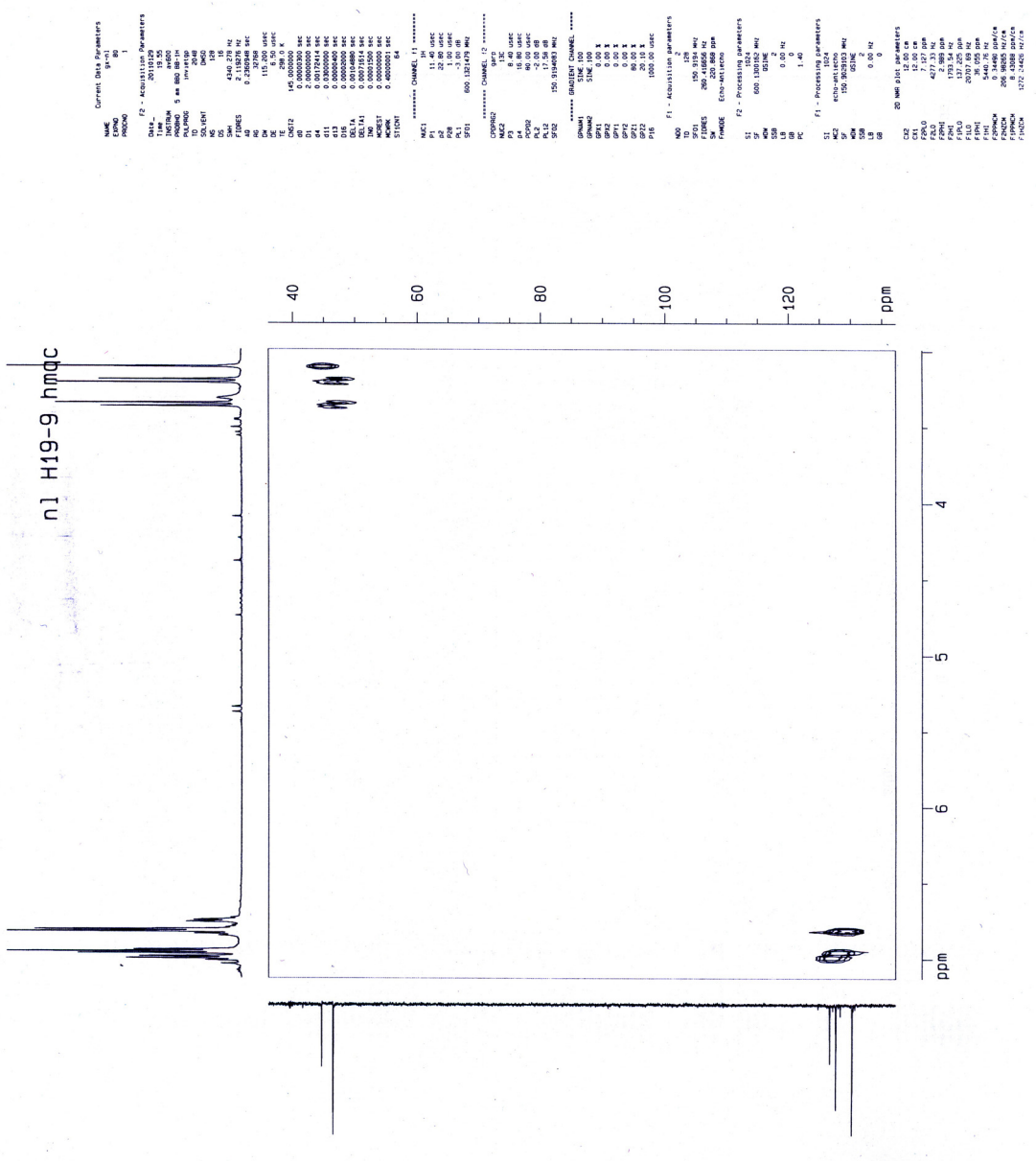

Figure S7. DEPT HMQC NMR spectrum of 7,23-($PhCH_2$)HC_{70} in CS_2 with DMSO-d_6 as the external lock.

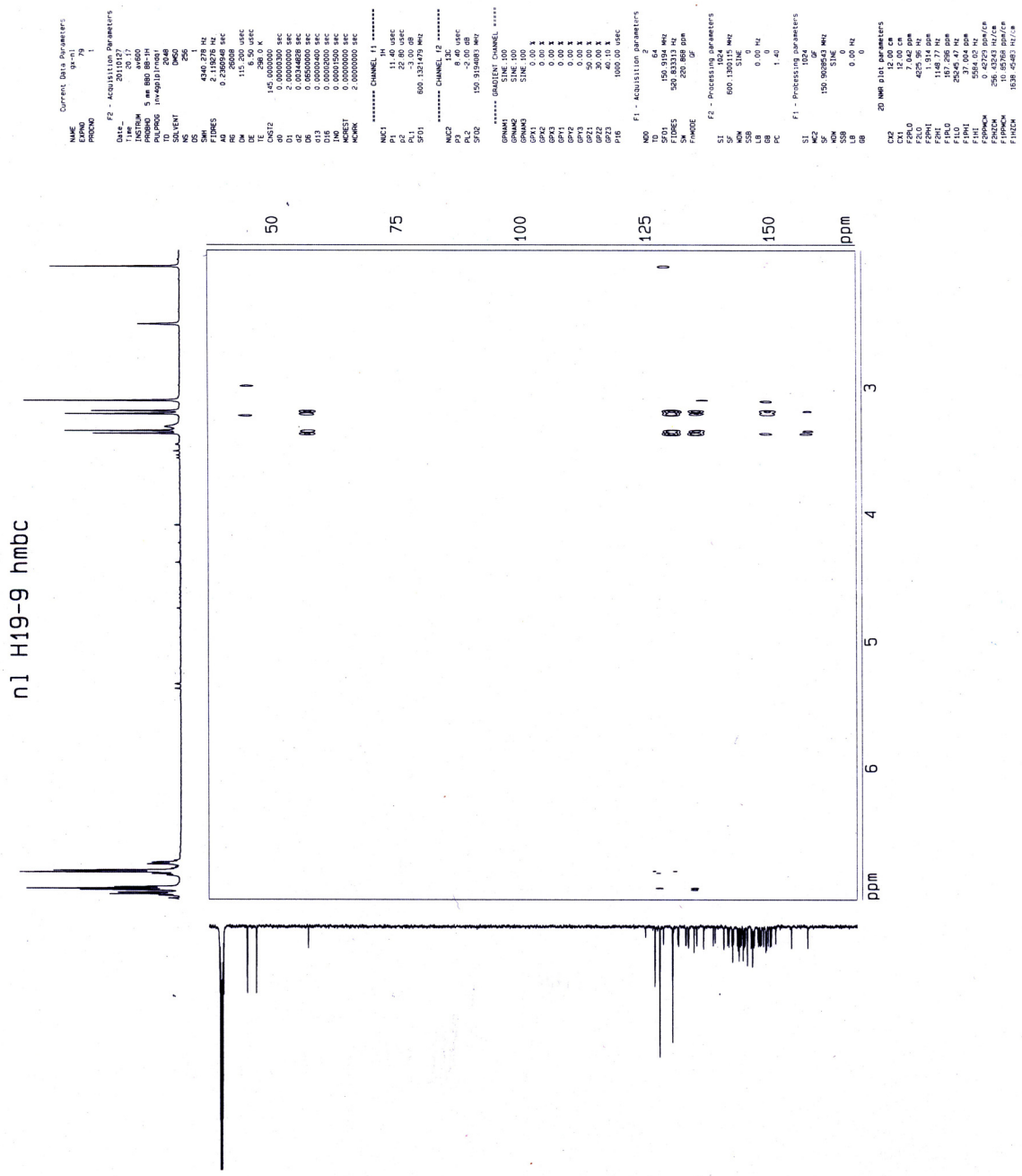

Figure S8. HMBC NMR spectrum of 7,23-($PhCH_2$)HC_{70} in CS_2 with DMSO-d_6 as the external lock.

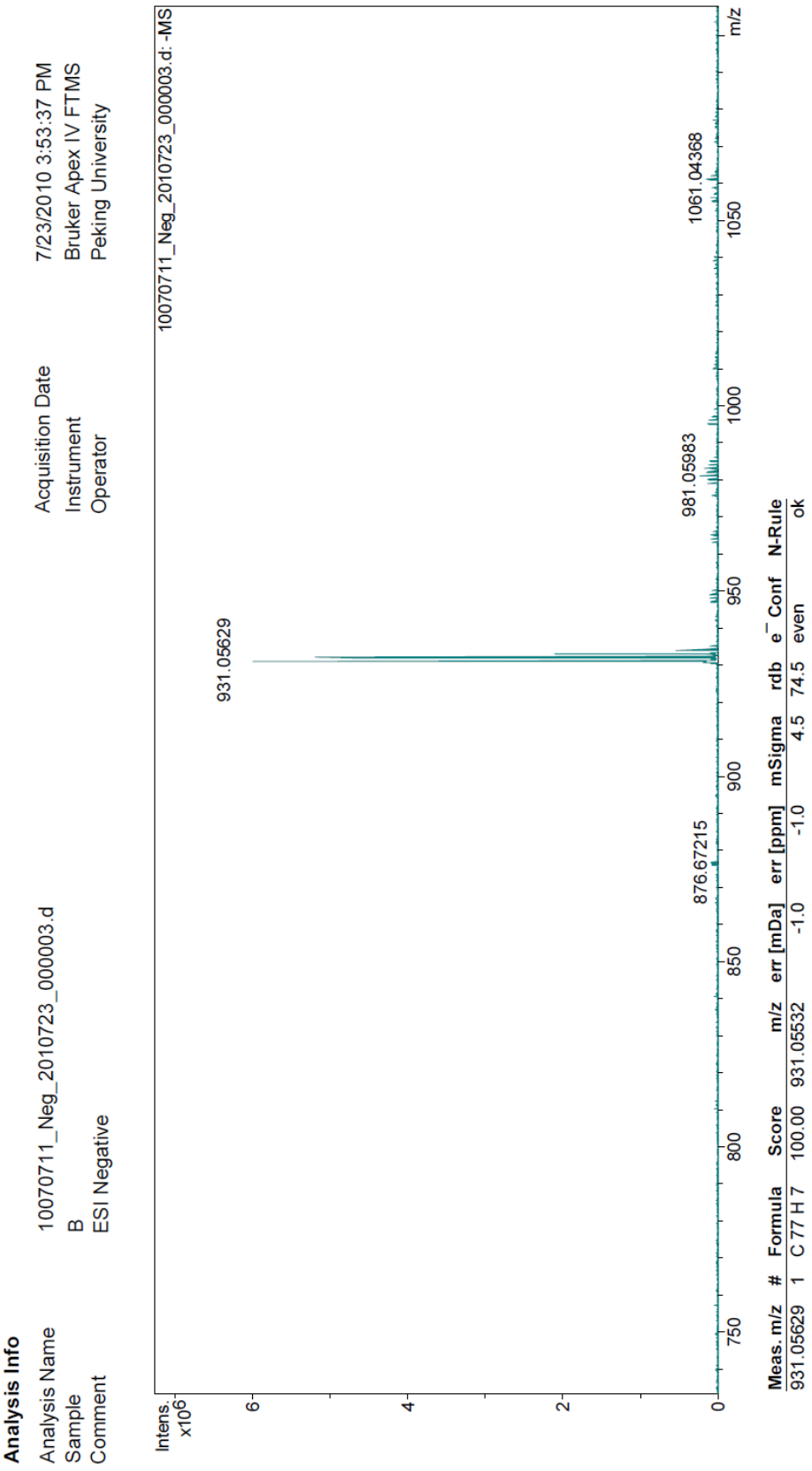

Figure S9. Negative ESI FT-ICR MS of 7,23-($PhCH_2$)HC_{70}.

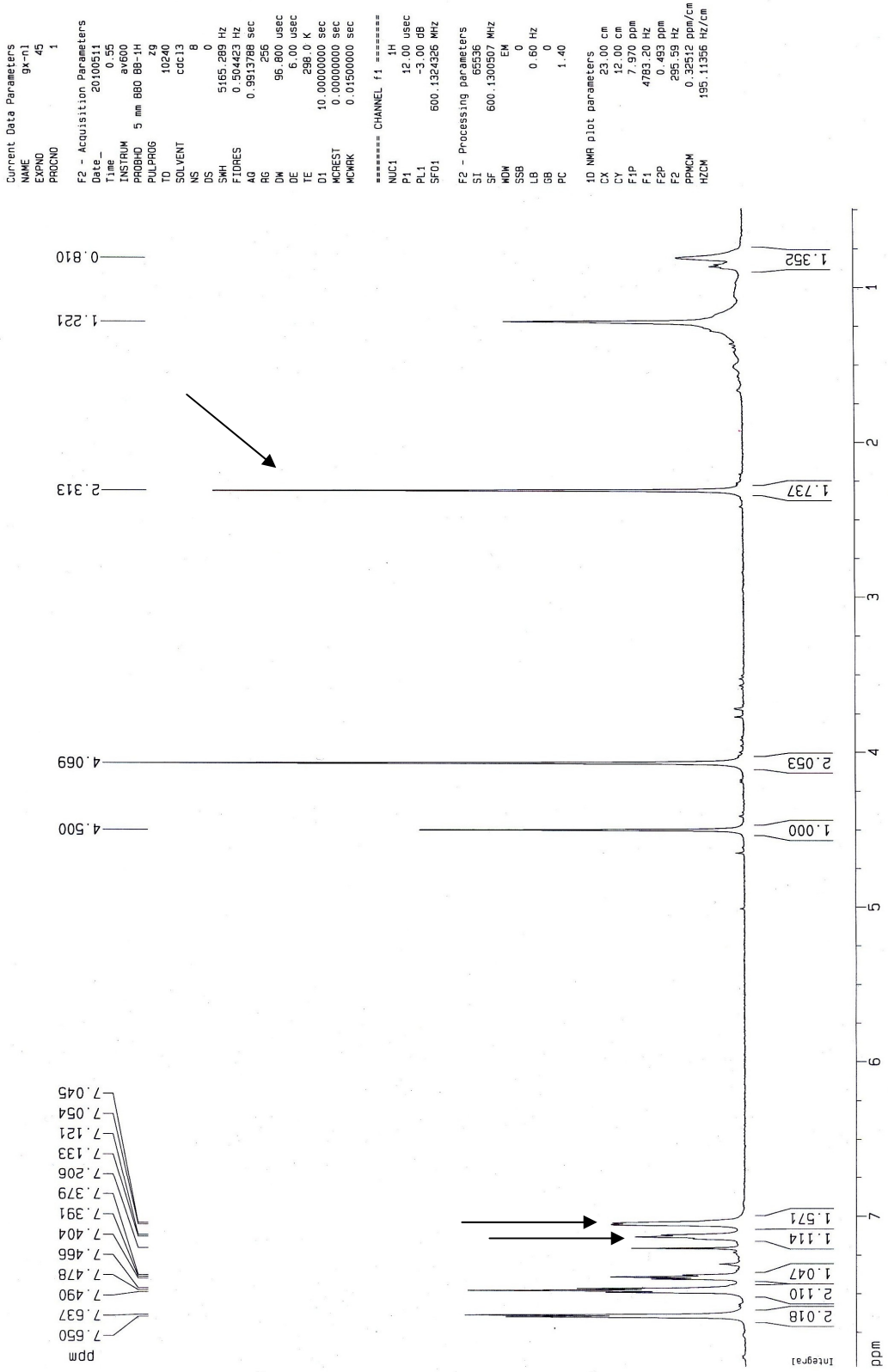

Figure S10. ^{1}H NMR spectrum of 1,2-H($PhCH_2$)C_{70} in CS_2/$CDCl_3$. Peaks labeled with arrows are due to the toluene residue used for HPLC purification.

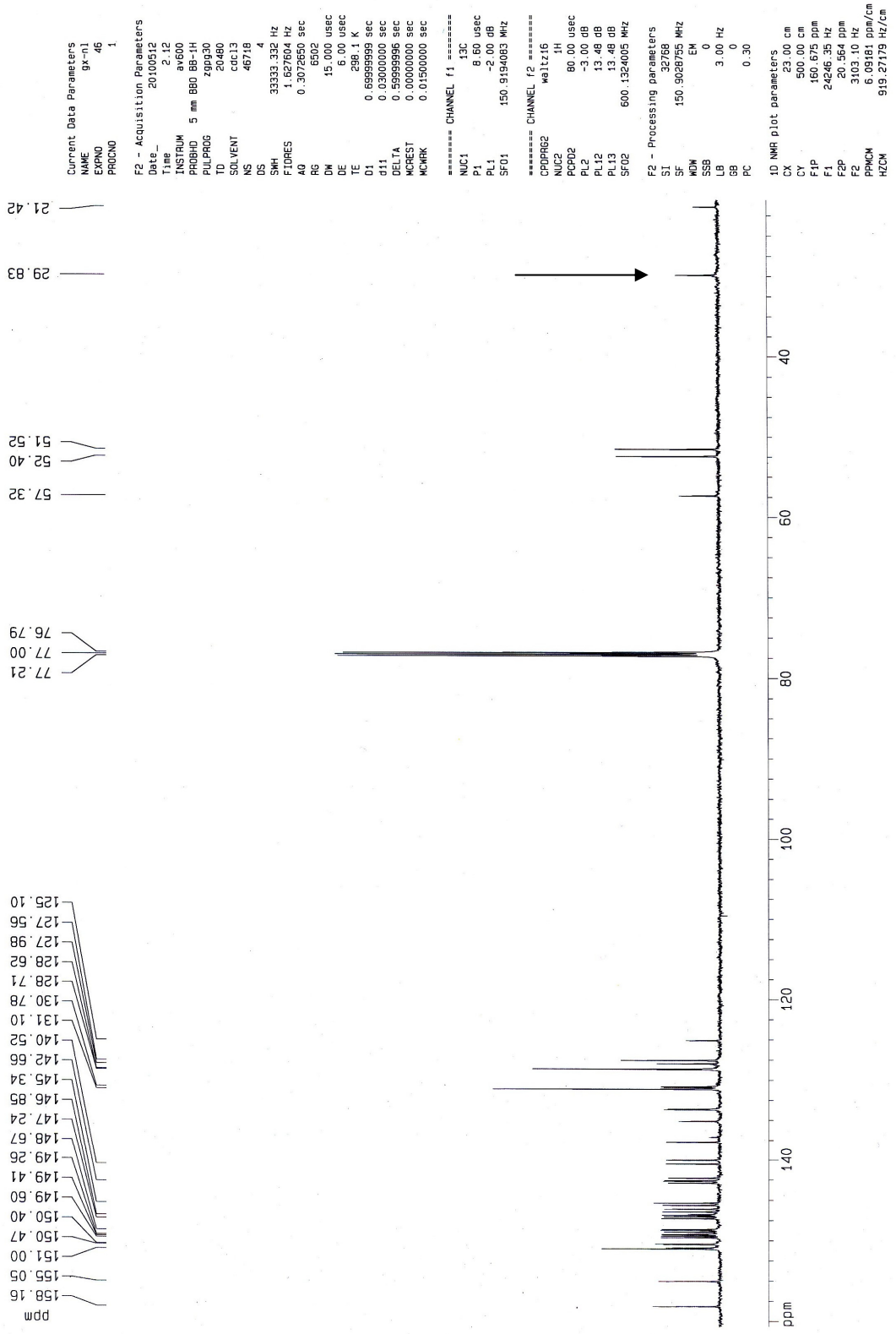

Figure S11. ^{13}C NMR spectrum of 1,2-H($PhCH_2$)C_{70} in CS_2/$CDCl_3$. The peak labeled with an arrow is due to the toluene residue used for HPLC purification.

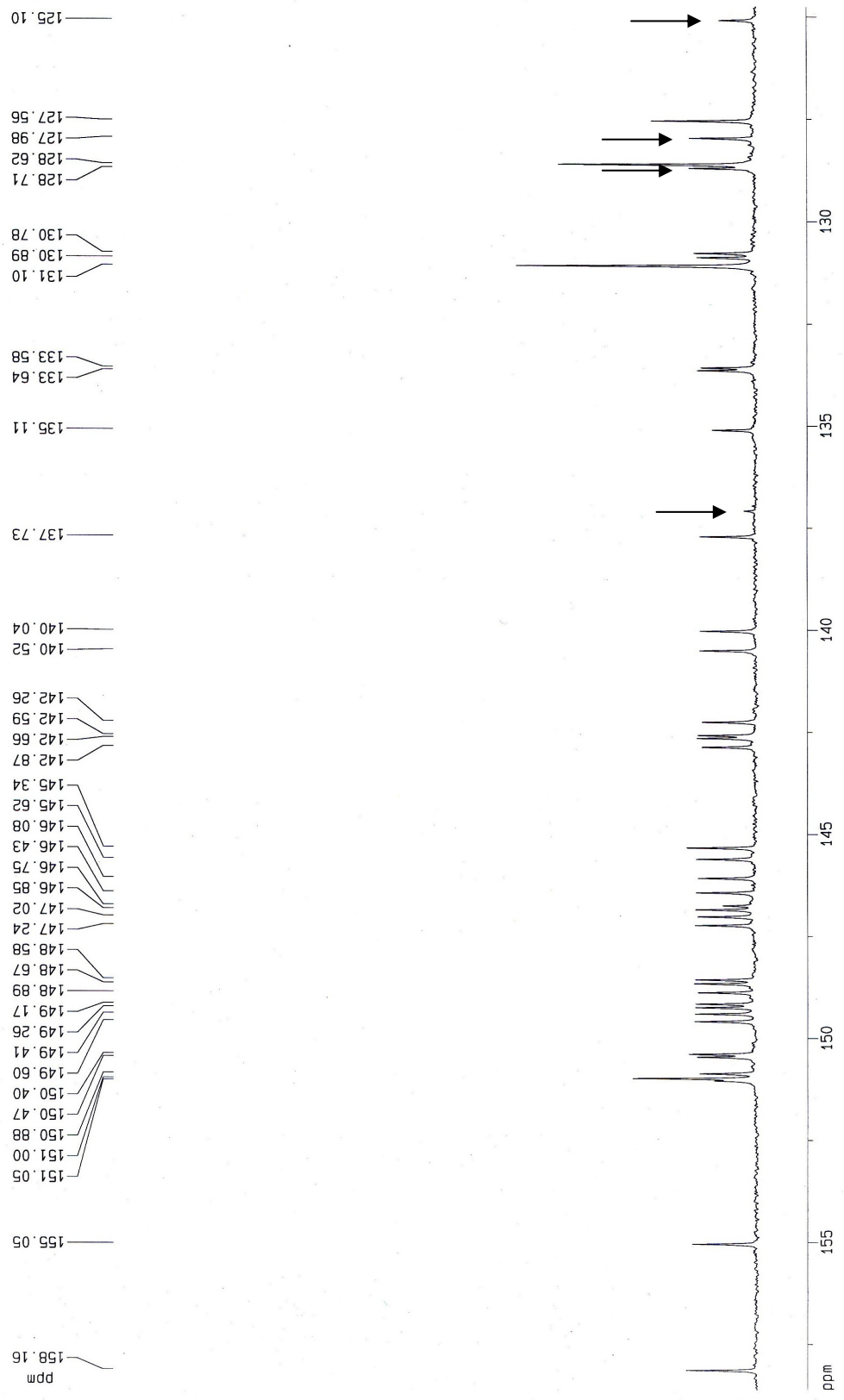

Figure S12. Expanded ^{13}C NMR spectrum for the sp^2 region of 1,2-H($PhCH_2$)C_{70} in CS_2/$CDCl_3$. Peaks labeled with arrows are from toluene residue used for HPLC purification.

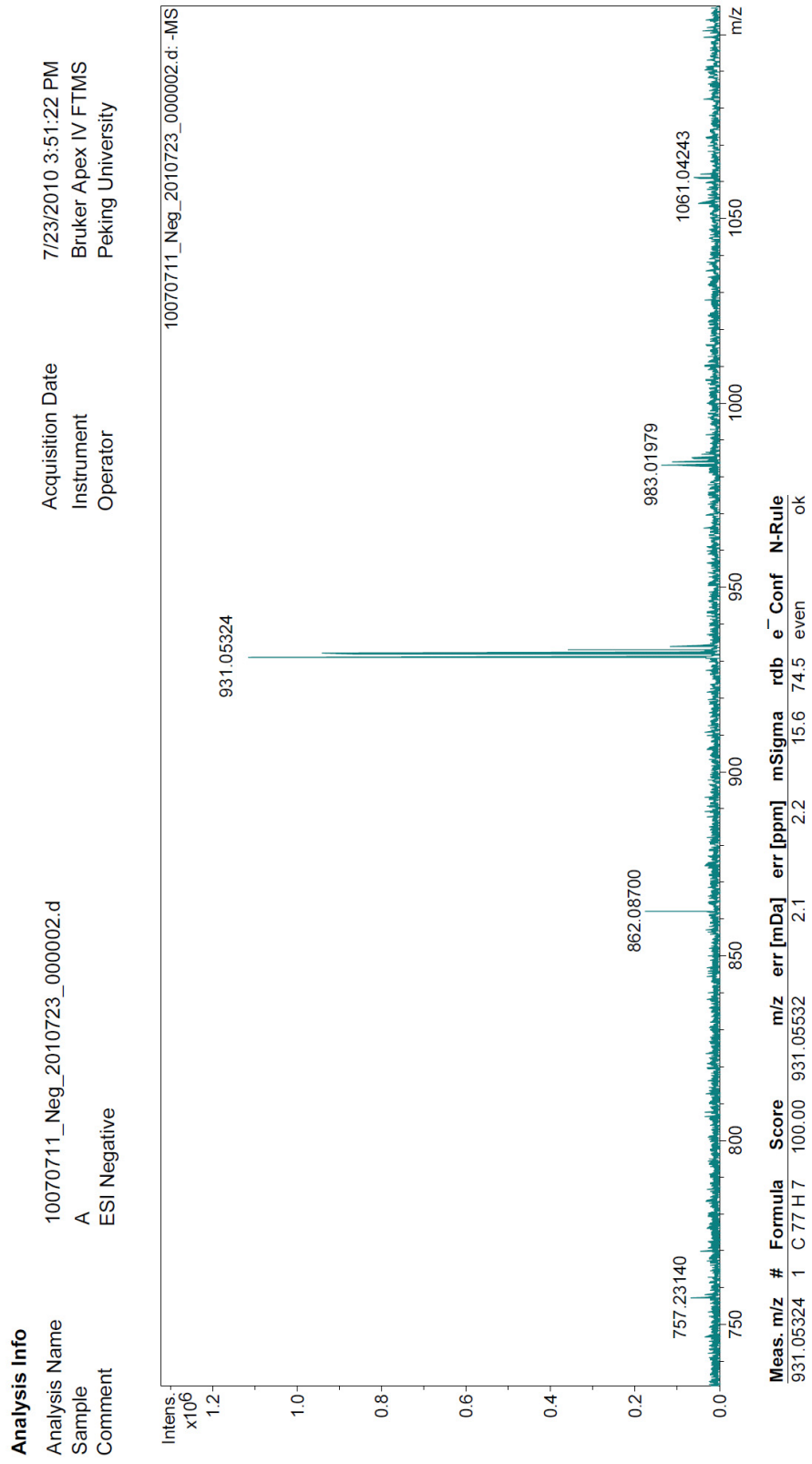

Figure S13. Negative ESI FT-ICR MS of 1,2-H($PhCH_2$)C_{70}.

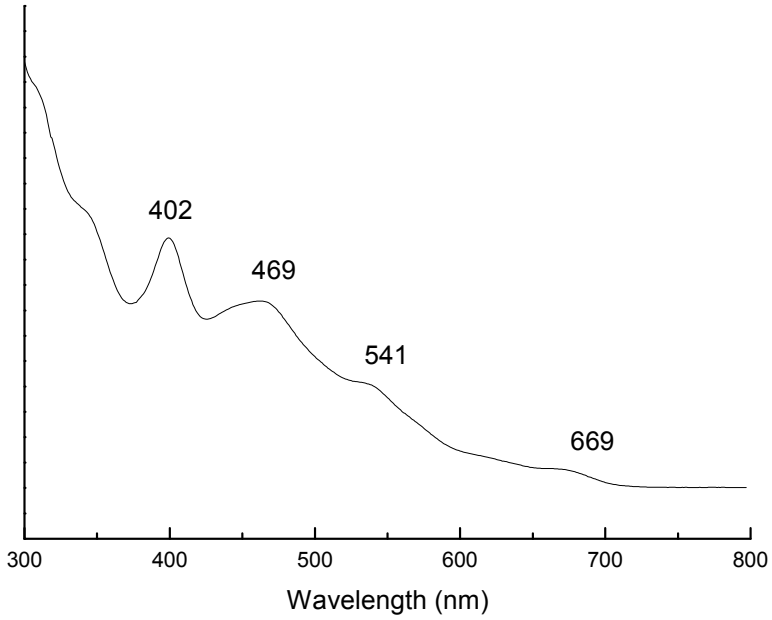

Figure S14. UV-vis spectrum of 1,2-H($PhCH_2$)C_{70} recorded in toluene solution.

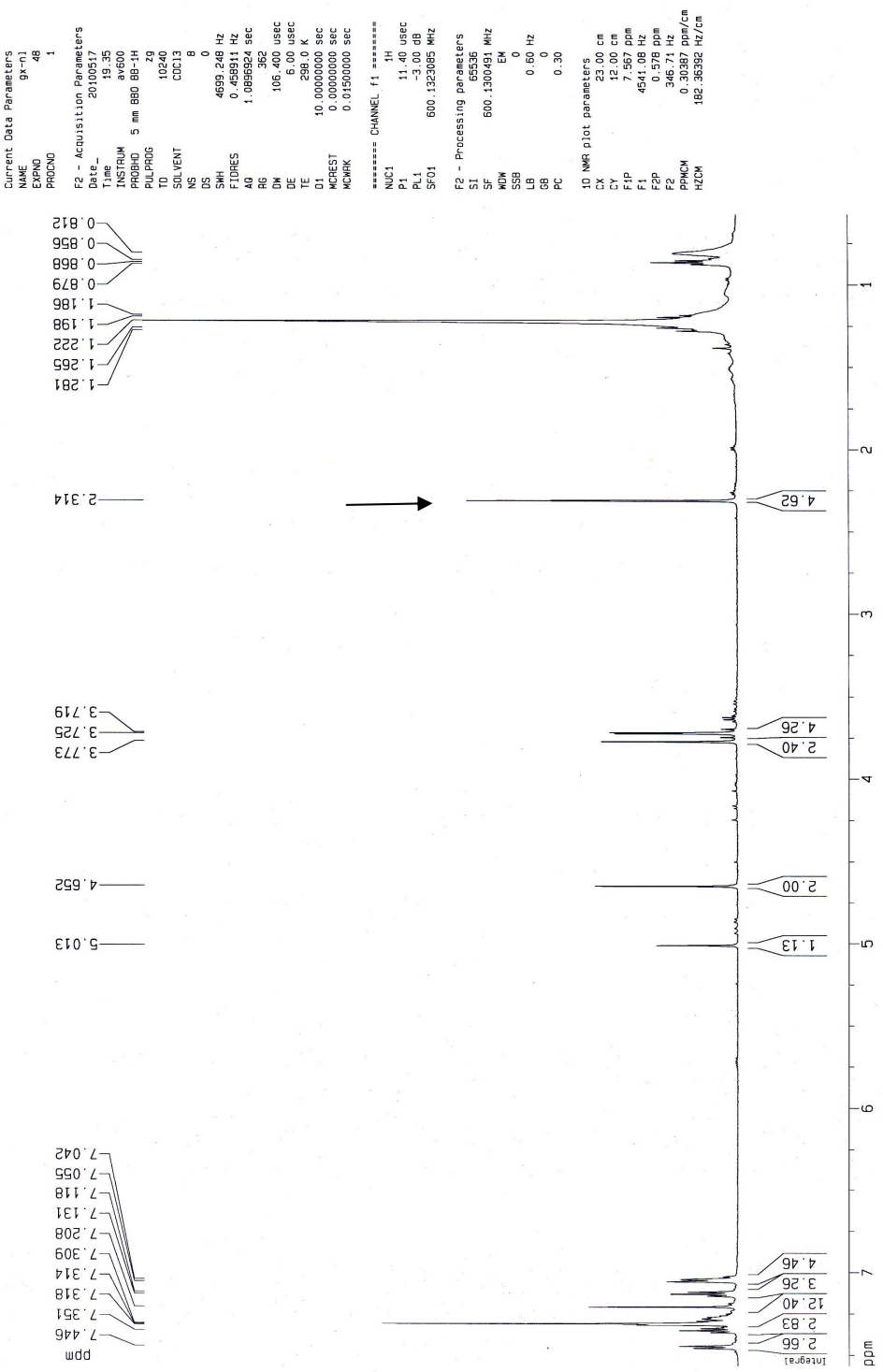

Figure S15. ^{1}H NMR spectrum of 2,1-H($PhCH_2$) C_{70} and 5,6-H($PhCH_2$)C_{70} mixture in CS_2/$CDCl_3$. The peak labeled with an arrow is from toluene residue used for HPLC purification.

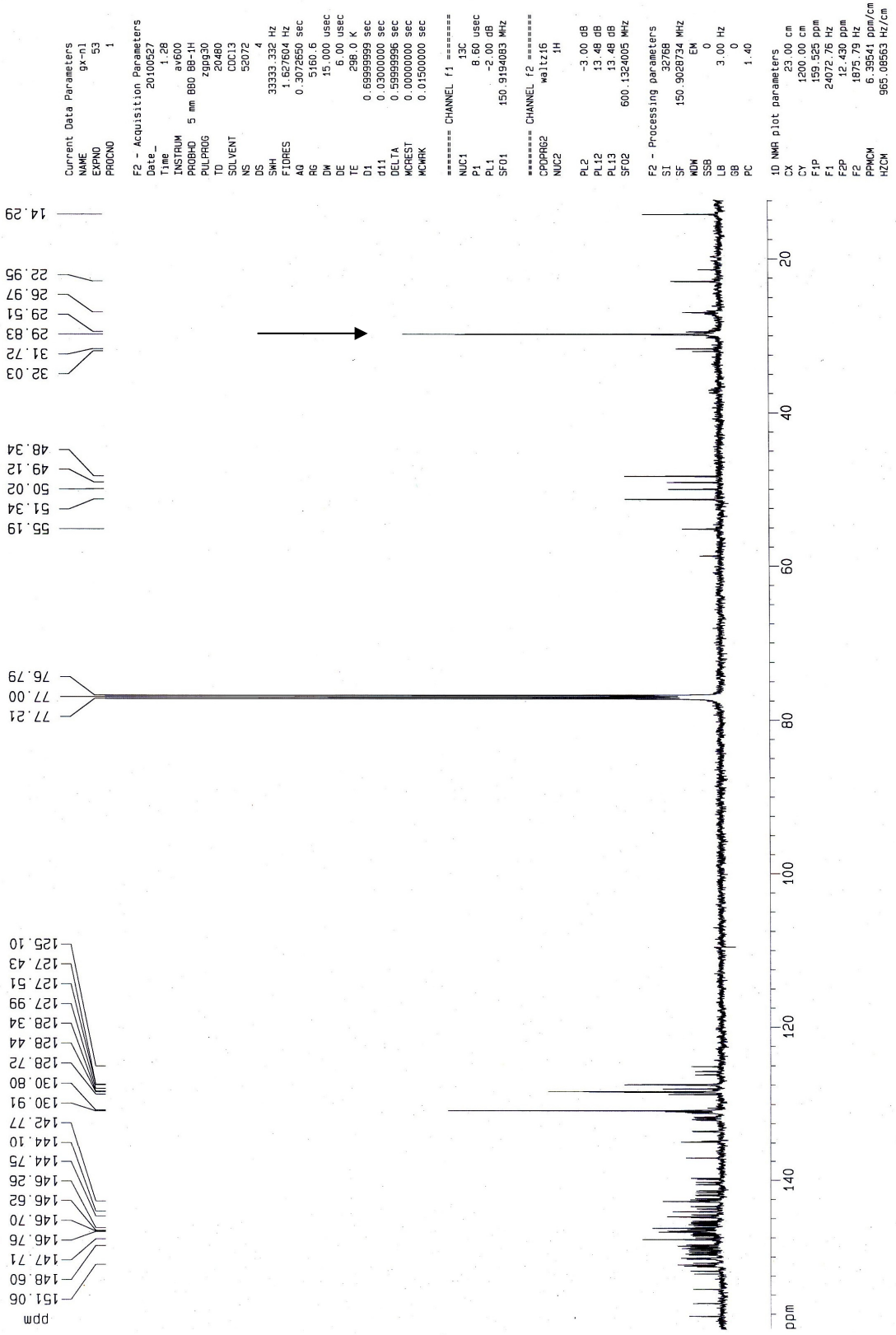

Figure S16. ^{13}C NMR spectrum of 2,1-H($PhCH_2$) C_{70} and 5,6-H($PhCH_2$)C_{70} mixture in CS_2/$CDCl_3$.

The peak labeled with an arrow is from toluene residue used for HPLC purification.

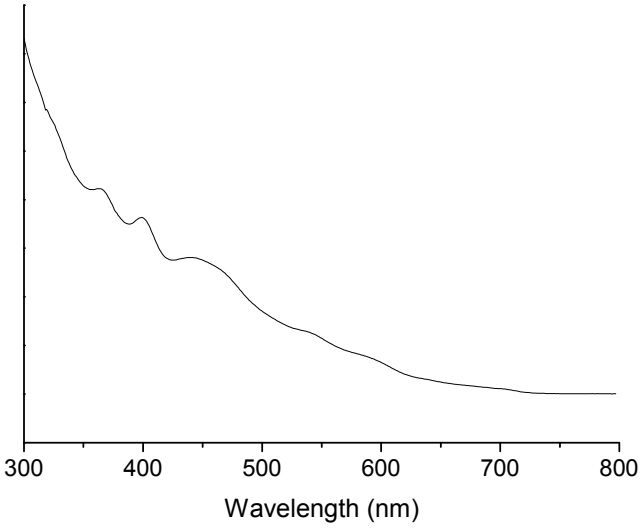

Figure S17. Uv-vis absorption spectrum of 2,1-H($PhCH_2$)C_{70} and 5,6-H($PhCH_2$)C_{70} mixture recorded in toluene.

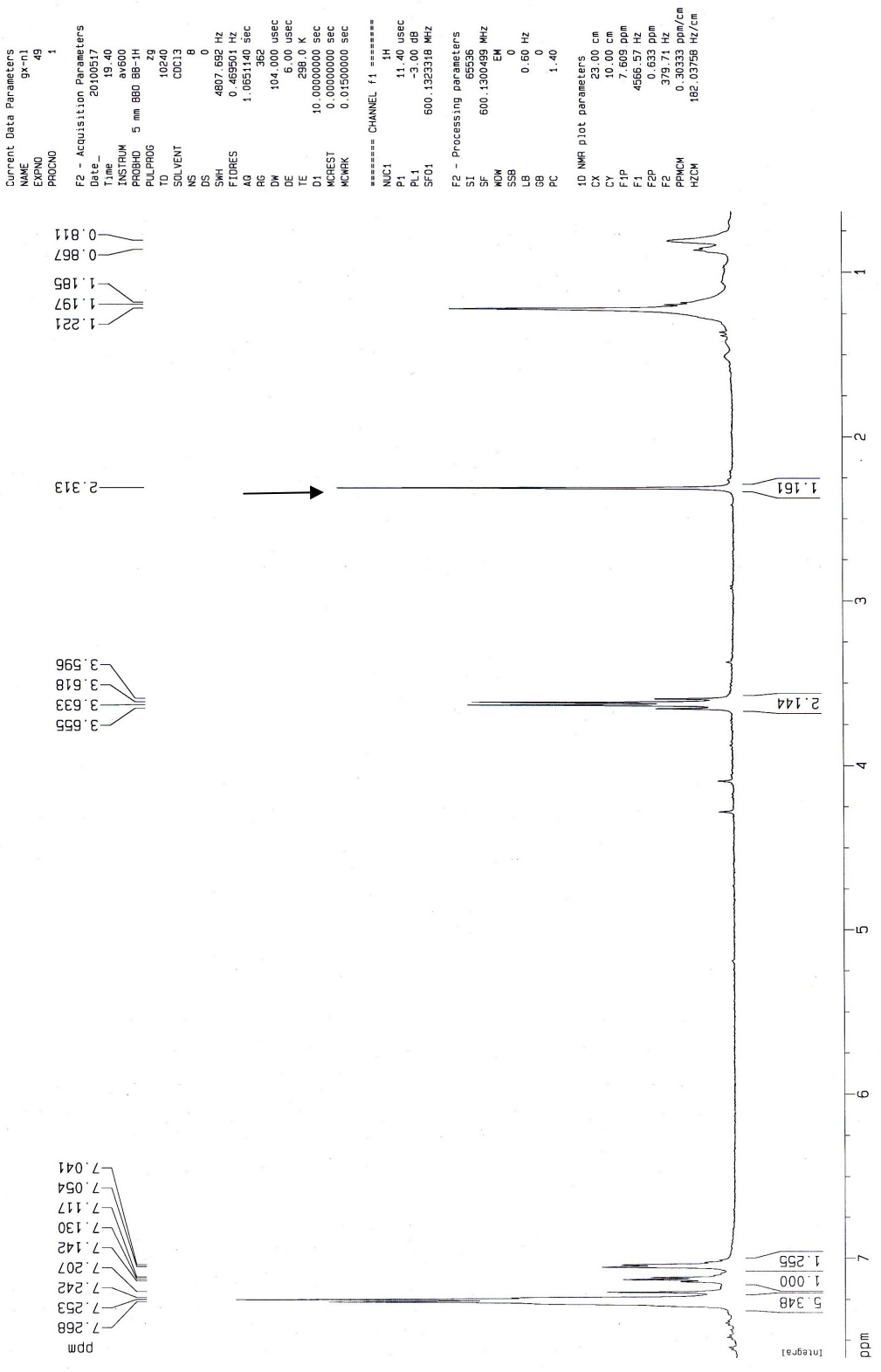

Figure S18. ^{1}H NMR spectrum of 7,23-$(PhCH_2)_2C_{70}$ in $CS_2/CDCl_3$. Peak labeled with arrows is from toluene residue used for HPLC purification.

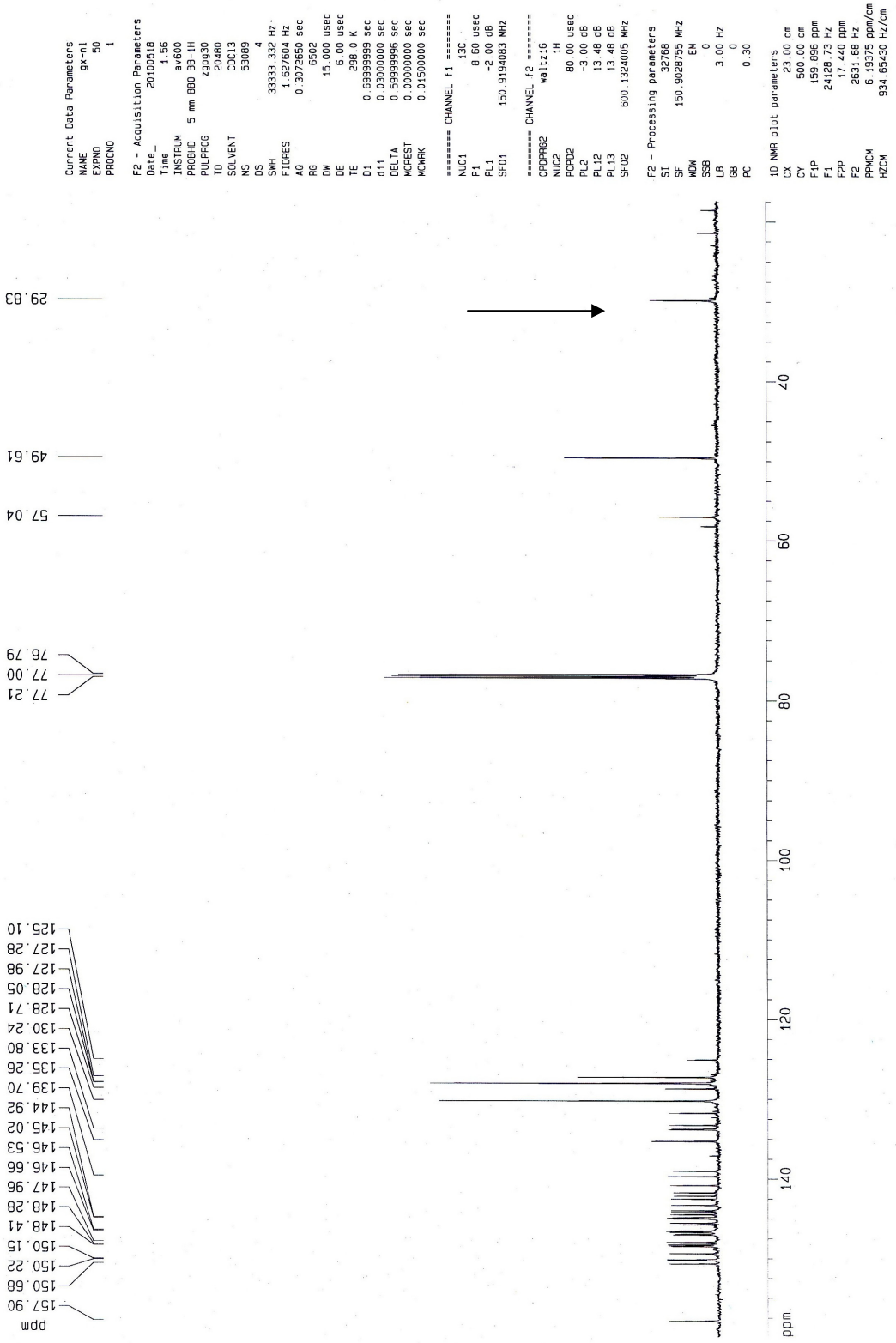

Figure S19. ^{13}C NMR spectrum of 7,23-$(PhCH_2)_2C_{70}$ in $CS_2/CDCl_3$. The peak labeled with an arrow is from toluene residue used for HPLC purification.

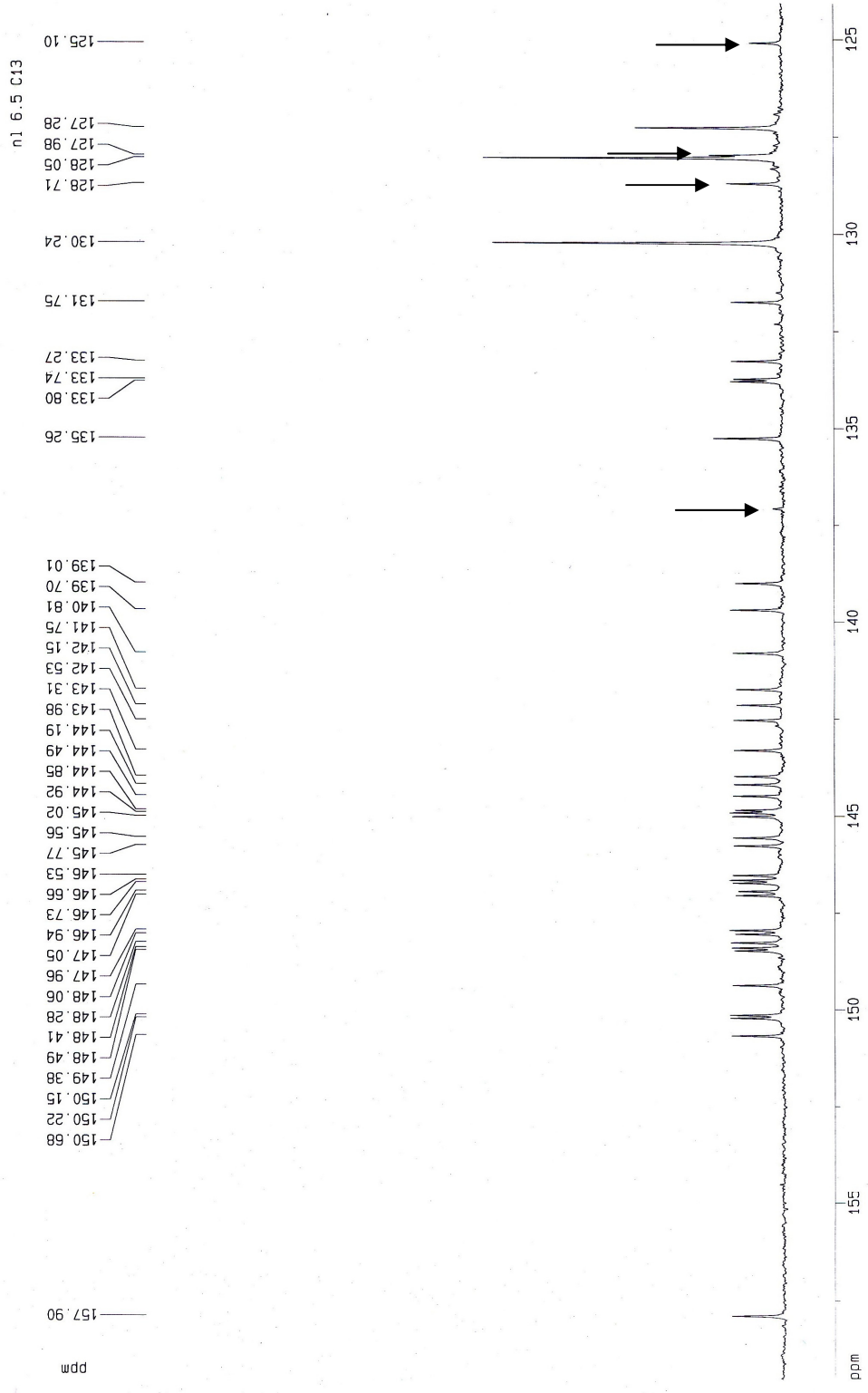

Figure S20. Expanded ^{13}C NMR spectrum for the sp^2 region of 7,23-$(PhCH_2)_2C_{70}$ in $CS_2/CDCl_3$. Peaks labeled with arrows are from the toluene residue used for HPLC purification.

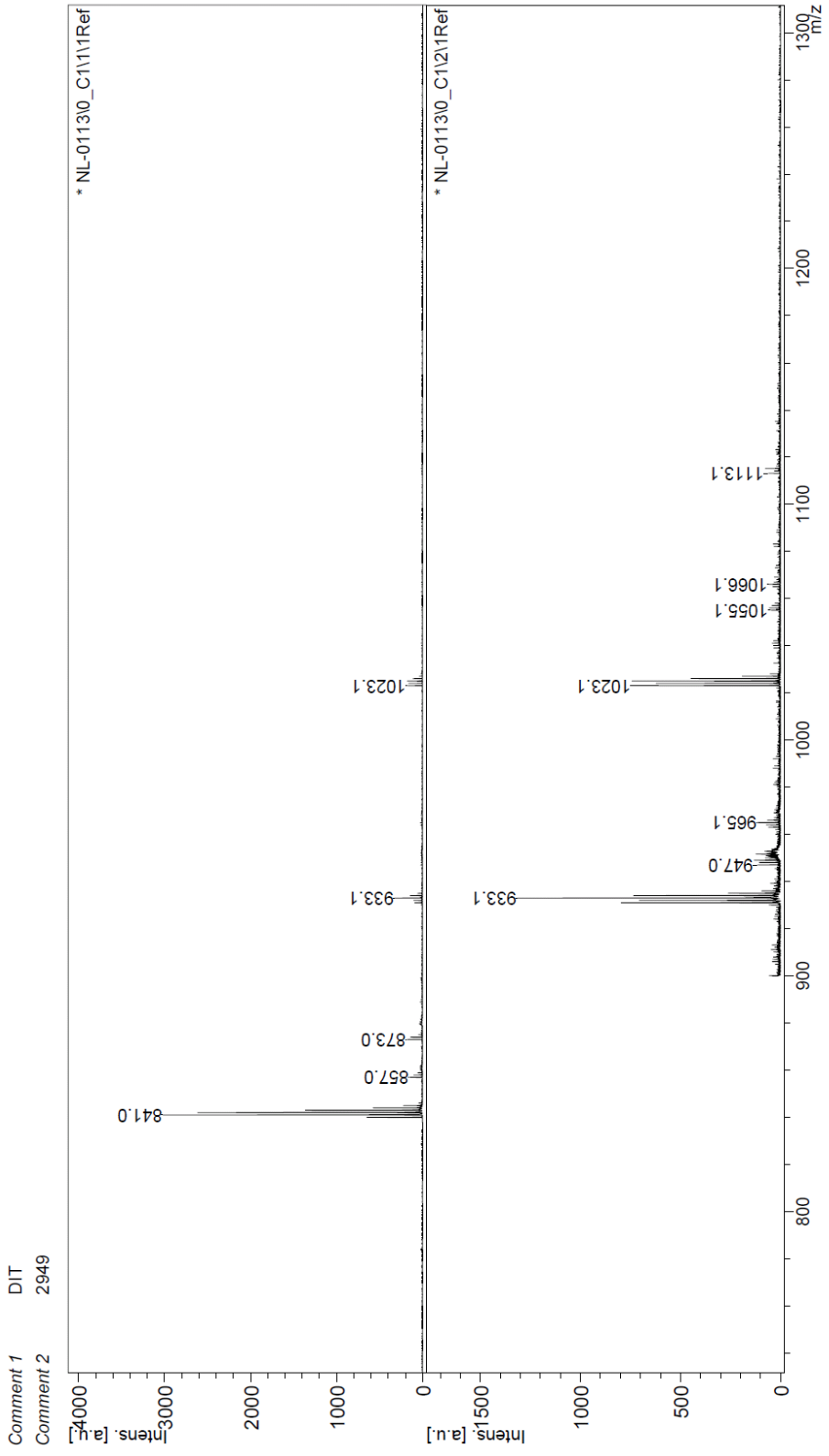

Figure S21. Positive MALDI MS of 7,23-$(PhCH_2)_2C_{70}$ with dithranol (DIT) as the matrix.

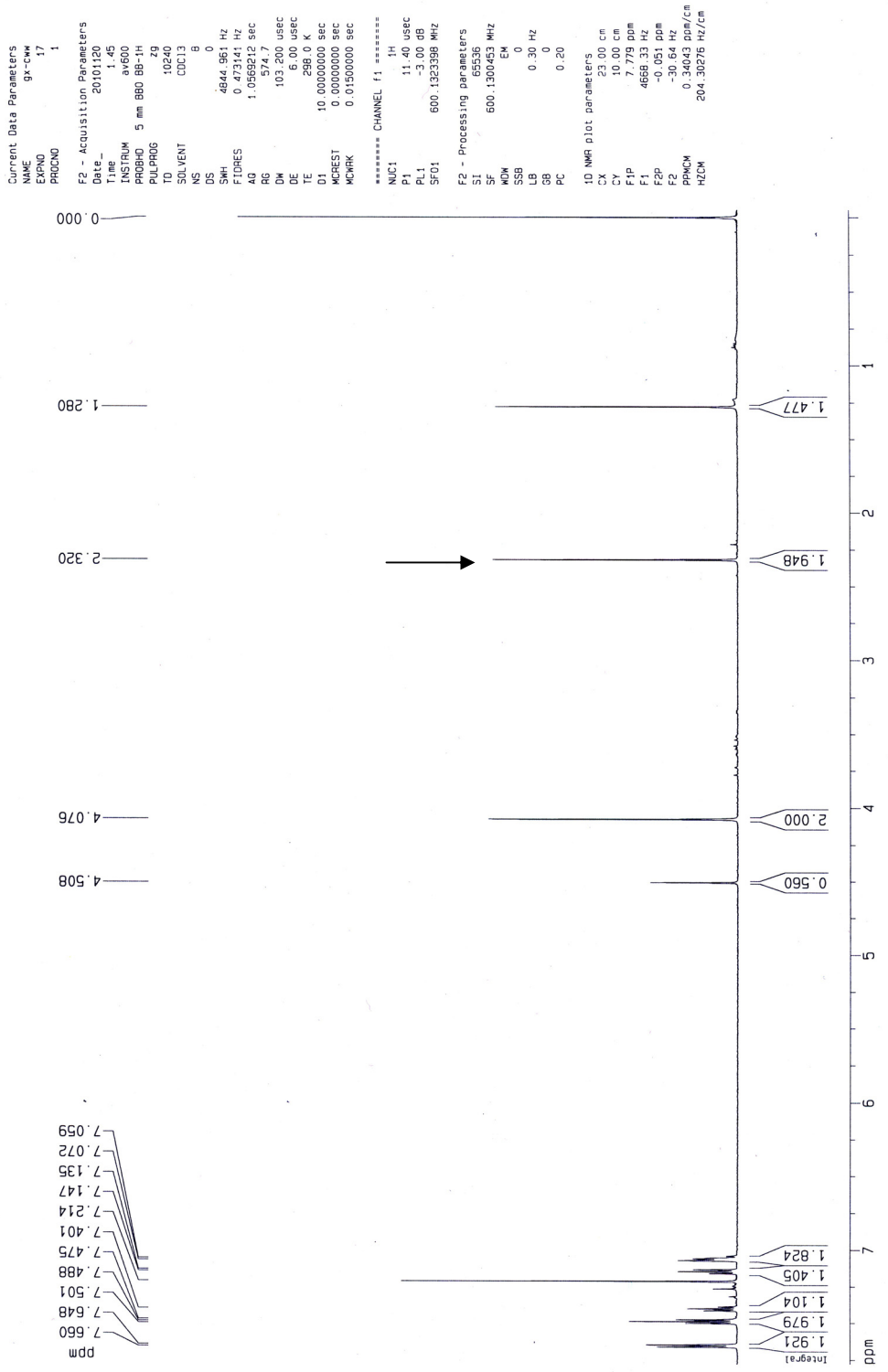

Figure S22. ^{1}H NMR spectrum of partial deuterated 1,2-H(PhCH$_2$)C$_{70}$ in CS$_2$/CDCl$_3$ obtained from the reaction of C_{70}^{2-} with benzyl bromide in DMF into which 100 μL D$_2$O was added. Peak labeled with arrows is from toluene residue used for HPLC purification.

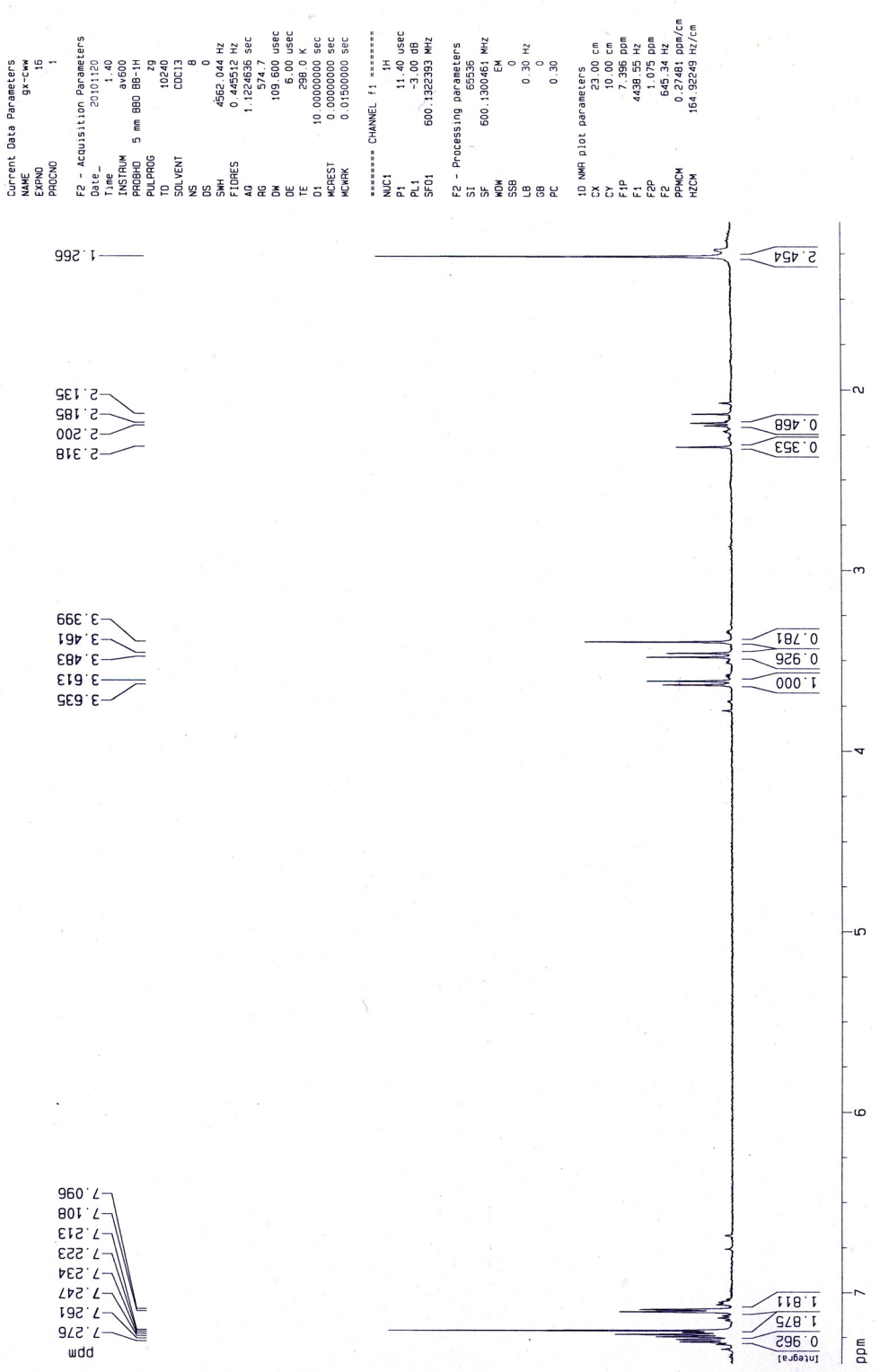

Figure S23. ^{1}H NMR spectrum of partial deuterated 7,23-($PhCH_2$)HC_{70} in CS_2/$CDCl_3$ obtained from the reaction of C_{70}^{2-} with benzyl bromide in DMF into which 100 μL D_2O was added.

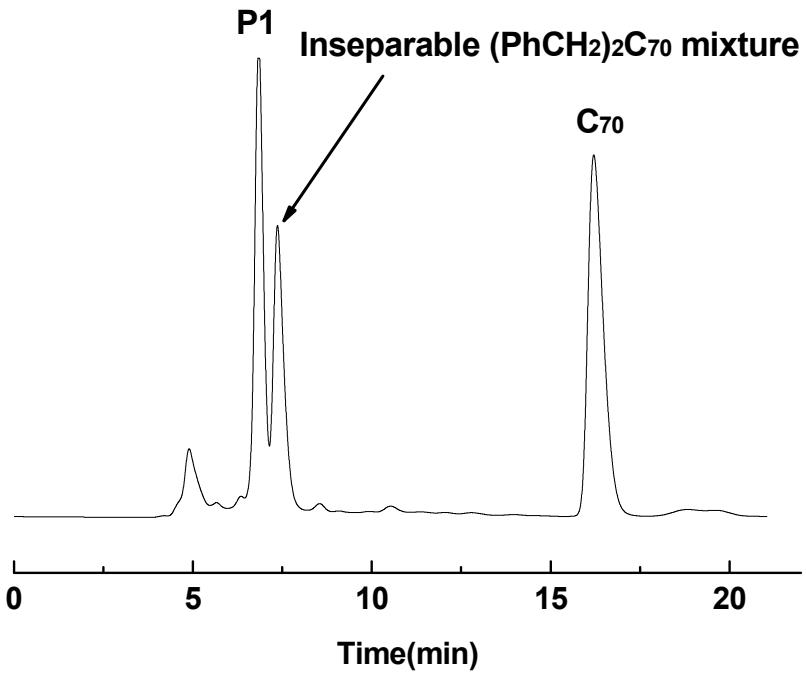

Figure S24. HPLC traces of the crude reaction mixture obtained from the reaction of C_{70}^{2-} with benzyl bromide in freshly distilled PhCN. The crude mixture was eluted by toluene over a semi-preparative Buckyprep column at a flow rate of 4.0 mL/min with the detector wavelength set at 380 nm.

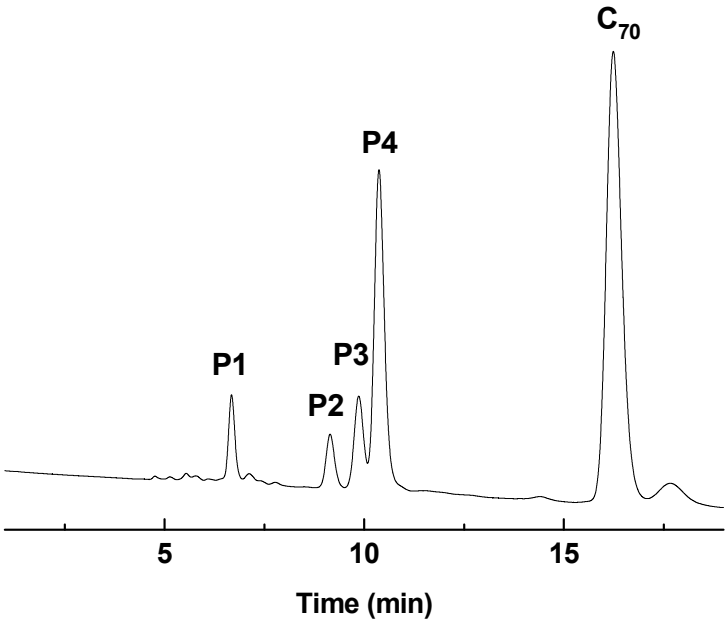

Figure S25. HPLC traces of the crude reaction mixture obtained from the reaction of C_{70}^{2-} with benzyl bromide in freshly distilled PhCN, where 30-fold benzyl bromide was first added into the C_{70}^{2-} solution, followed by addition of 200 μL H_2O after C_{70}^{2-} reacted with benzyl bromide for about 5 min. The crude mixture was eluted by toluene over a semi-preparative Buckyprep column at a flow rate of 4.0 mL/min with the detector wavelength set at 380 nm.

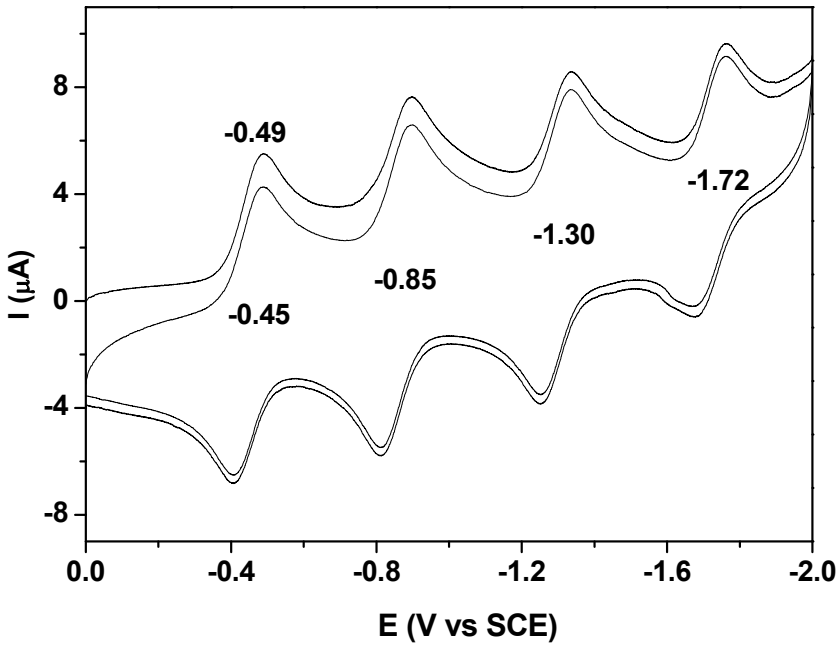

Figure S26. Cyclic voltammogram of C_{70} in PhCN containing 0.1 M TBAP. Scan rate = 0.1 V/s.

Cartesian coordinates, total energies and lowest frequencies of the reported stationary points for 1-$PhCH_2C_{70}^-$, 2-$PhCH_2C_{70}^-$, 5-$PhCH_2C_{70}^-$, 7-$PhCH_2C_{70}^-$, 21-$PhCH_2C_{70}^-$ intermediates and **2**, **4**, **5**, **6**, **7** obtained at B3LYP/6-31G level.

Geometry of 1-$PhCH_2C_{70}^-$

-1 1

C	-2.01970500	2.93241000	1.14600500
C	-0.91989400	3.81835000	0.71610200
C	-0.91989000	3.81835400	-0.71609000
C	-2.01969800	2.93241700	-1.14600500
C	2.93463400	-3.28304500	1.17915900
C	2.26079000	-3.81951800	-0.00000700
C	2.93464200	-3.28303700	-1.17916600
C	4.02298400	-2.42583600	-0.72763700
C	4.02297900	-2.42584000	0.72764300
C	-1.85111100	2.15827800	2.31472500
C	0.29397200	3.82997100	1.42757400
C	0.29398100	3.82998000	-1.42755400
C	-1.85109700	2.15829200	-2.31472900
C	2.18204100	-2.91981700	2.30207200
C	0.87040300	-3.96371500	-0.00001200
C	2.18205600	-2.91980300	-2.30208100
C	4.30687200	-1.23923400	-1.42194300
C	4.30686300	-1.23924300	1.42195700
C	-2.31481400	0.76747100	2.27750400
C	0.47147900	2.99671000	2.59178800
C	1.54994100	3.82945800	-0.69592200

C	-0.58270800	2.15852100	-2.99571900
C	-2.98151100	0.25368200	-1.17989500
C	2.47684800	-1.68489000	3.01347500
C	0.09109600	-3.58218800	1.17027700
C	0.73513100	-3.07014000	-2.29500300
C	3.51327400	-0.86369800	-2.58043500
C	4.59636100	-0.01517400	0.69532300
C	0.73511600	-3.07015400	2.29498400
C	3.51325800	-0.86371400	2.58044600
C	4.59636600	-0.01516900	-0.69529900
C	2.47686700	-1.68487200	-3.01347500
C	0.09110300	-3.58218000	-1.17030300
C	-0.58272600	2.15850300	2.99572300
C	-2.98151800	0.25367500	1.17987200
C	-2.31480000	0.76748500	-2.27751900
C	0.47149500	2.99672600	-2.59177200
C	1.54993700	3.82945400	0.69595000
C	-1.34761100	-0.05328600	2.98975900
C	1.83132300	2.47738500	2.57972800
C	2.50693300	3.00295900	-1.41783800
C	-0.28123100	0.80092700	-3.43268000
C	-2.64417500	-1.06877800	-0.72075600
C	1.22297700	-1.09498000	3.45720700
C	-1.15605900	-2.98902400	0.72021000
C	0.15199100	-1.95064100	-3.01504200
C	3.34060100	0.58319800	-2.57721800
C	4.01376300	1.10879200	1.42133200
C	0.15197200	-1.95065900	3.01502600
C	3.34058400	0.58318200	2.57723700

C	4.01377200	1.10880000	-1.42130500
C	1.22299800	-1.09495800	-3.45721100
C	-1.15605400	-2.98902000	-0.72024000
C	-0.28125200	0.80090600	3.43267800
C	-2.64417900	-1.06878200	0.72072800
C	-1.34759200	-0.05326800	-2.98977300
C	1.83133900	2.47740100	-2.57970700
C	2.50692400	3.00295000	1.41786700
C	-1.11367300	-1.41271600	2.64408000
C	2.15826300	1.19061500	3.09513400
C	3.50791400	2.25358300	-0.73912600
C	1.05559900	0.31724700	-3.54108700
C	-1.78858700	-1.94640800	-1.45572600
C	1.05557700	0.31722600	3.54109000
C	-1.78859700	-1.94641700	1.45569800
C	-1.11365600	-1.41270000	-2.64410100
C	2.15828300	1.19063400	-3.09511900
C	3.50790900	2.25357800	0.73915600
C	-2.73003900	2.46410400	-0.00000400
C	-3.48033100	1.12970900	-0.00001000
C	-5.04309000	1.35606900	-0.00001100
H	-5.26484800	1.96980100	0.88132300
H	-5.26485000	1.96979900	-0.88134500
C	-5.90494500	0.11297200	-0.00000600
C	-6.31257600	-0.48345600	-1.20691800
C	-6.31256900	-0.48344800	1.20691400
C	-7.10027400	-1.63956900	-1.20924900
H	-6.00342100	-0.03790800	-2.14809200
C	-7.10026700	-1.63956000	1.20925800

H	-6.00340600	-0.03789200	2.14808100
C	-7.49800000	-2.22213200	0.00000800
H	-7.40204700	-2.08469600	-2.15306500
H	-7.40203400	-2.08468100	2.15307900
H	-8.10930800	-3.11986000	0.00001400

Total energy = –2937.6019 a.u.

Lowest frequency = 20.2 cm^{-1}

Geometryof 2-$PhCH_2C_{70}^-$

-1 1

C	2.69592300	1.99560300	-1.26386200
C	2.25978900	2.85273800	-0.19292000
C	2.58477200	2.21325800	1.07231500
C	3.23159500	0.95421600	0.79903500
C	-4.50118000	-1.43865200	-1.15501100
C	-3.92762200	-2.63517700	-0.55384800
C	-3.97829400	-2.47420200	0.89280400
C	-4.59869300	-1.18219800	1.18498400
C	-4.92095200	-0.54440000	-0.07648800
C	1.89451800	1.86341800	-2.39143600
C	1.08476800	3.62427600	-0.30853200
C	1.71992500	2.36834800	2.17557300
C	2.91143300	-0.14646700	1.58551200
C	3.06348100	-0.49251200	-1.25452200
C	-3.93488700	-0.90771100	-2.31957200
C	-2.81394000	-3.24695100	-1.14774500
C	-2.91404700	-2.92943600	1.67916300

C	-4.11279300	-0.41177800	2.25363100
C	-4.74553800	0.84124100	-0.22395000
C	1.65708300	0.55879800	-3.01413600
C	0.26921400	3.49406700	-1.48797900
C	0.48680200	3.13152700	2.03426700
C	1.98811200	-0.01093600	2.70079600
C	2.71503100	-1.57867800	-0.40228500
C	-3.75349600	0.53023200	-2.46086700
C	-2.23139100	-2.68970100	-2.35675200
C	-1.75933800	-3.55812700	1.05729100
C	-3.00839000	-0.89040600	3.06510000
C	-4.24521200	1.63491000	0.88621300
C	-2.77617000	-1.54296300	-2.92701100
C	-4.15662200	1.38427200	-1.43402500
C	-3.93608600	1.02231900	2.09749500
C	-2.41508000	-2.12114200	2.78271200
C	-1.71292800	-3.71760000	-0.32462400
C	0.65824300	2.62083000	-2.50497300
C	2.20978000	-0.57343200	-2.39064900
C	2.67956500	-1.46833400	0.99705100
C	1.41457600	1.22617700	2.99741800
C	0.17763100	3.74381200	0.82468500
C	0.29541500	0.52831200	-3.47856900
C	-1.13229500	3.55519900	-1.09830700
C	-0.56008300	2.47177200	2.79760600
C	1.20674100	-1.22089600	2.80526500
C	1.70713000	-2.41801900	-1.06341600
C	-2.51383100	0.77470800	-3.17165400
C	-0.78446900	-2.83832600	-2.28663300

C	-0.56362800	-3.15701600	1.78515200
C	-2.16860800	0.24401100	3.41772100
C	-3.37362500	2.67646900	0.35966400
C	-1.90152300	-0.50632200	-3.45703400
C	-3.31458400	2.51394300	-1.07161400
C	-2.74336300	1.42777100	2.82917500
C	-0.97517500	-2.27280000	2.85543900
C	-0.46486200	-3.47225500	-1.03355700
C	-0.32207000	1.80709900	-3.18353900
C	1.39128900	-1.79108900	-2.30354600
C	1.62645100	-2.10915200	1.73901200
C	0.01248800	1.28804700	3.38529200
C	-1.18977700	3.71857300	0.33154100
C	-0.49297200	-0.66962400	-3.48319300
C	-2.13259900	2.82545100	-1.80305300
C	-1.92388300	2.50060400	2.38025900
C	-0.13785700	-1.20095800	3.27594400
C	0.73521700	-3.15967200	-0.33502500
C	-1.71216200	1.91707500	-2.89013600
C	0.08864300	-1.87737800	-2.87010300
C	0.68381500	-3.00122800	1.12920000
C	-0.75951900	0.10582500	3.57547800
C	-2.25187900	3.15029700	1.09512800
C	3.58282200	0.84150200	-0.71233500
C	5.10245100	1.11662500	-1.02646300
H	5.20045600	1.12709600	-2.11894000
H	5.33512100	2.12749200	-0.66790800
C	6.07443400	0.12283800	-0.42993300
C	6.68367300	0.36917400	0.81311300

C	6.38668900	-1.07345500	-1.10056000
C	7.58022600	-0.54899400	1.37010000
H	6.44773300	1.28565100	1.34652800
C	7.28149600	-1.99461400	-0.54587400
H	5.91471300	-1.28265800	-2.05523900
C	7.88324300	-1.73505600	0.69113600
H	8.03902000	-0.33941400	2.33215700
H	7.50638400	-2.91447200	-1.07798400
H	8.57831700	-2.44977400	1.12215100

Total energy = –2937.6136 a.u.

Lowest frequency = 21.9 cm^{-1}

Geometry of 5-$PhCH_2C_{70}^-$

-1 1

C	-2.01010100	2.92313900	1.26079400
C	-0.93714600	3.79137500	0.80335000
C	-0.96502100	3.82059800	-0.65710600
C	-2.05238100	2.98720200	-1.10568100
C	2.96136200	-3.27312400	1.12382800
C	2.27466400	-3.79281700	-0.05062400
C	2.92483900	-3.23517200	-1.23181100
C	4.02366900	-2.38259500	-0.78537600
C	4.04020600	-2.40150400	0.66898200
C	-1.81733400	2.10610700	2.38467100
C	0.28484600	3.80835600	1.48976400
C	0.25942300	3.86419100	-1.36751400
C	-1.86521800	2.13881100	-2.21000900

C	2.22557500	-2.93232200	2.26641900
C	0.88186900	-3.94542400	-0.03318900
C	2.15381500	-2.85816400	-2.33529600
C	4.28569400	-1.18781300	-1.46975100
C	4.33181300	-1.22786400	1.38072900
C	-2.28401600	0.74090800	2.36106700
C	0.48536200	2.94287300	2.64228900
C	1.52158300	3.84773200	-0.64031500
C	-0.59553100	2.18039000	-2.94783700
C	2.52647100	-1.71046500	2.99408700
C	0.12364300	-3.58420700	1.15327000
C	0.70738600	-3.01304600	-2.30886900
C	3.49790000	-0.80347800	-2.62522000
C	4.60721100	0.00630700	0.67010500
C	0.77953400	-3.08748000	2.27553100
C	3.55249500	-0.87679200	2.55957900
C	4.58239700	0.03061300	-0.72420200
C	2.43389400	-1.61359300	-3.04139000
C	0.08602400	-3.54945500	-1.18366300
C	-0.54109100	2.11340900	3.08251900
C	-2.91737600	0.25677100	1.21657300
C	0.43663600	3.02811500	-2.52583500
C	1.53596700	3.83021800	0.75156500
C	-1.30933300	-0.09181000	3.05839600
C	1.85488900	2.45140300	2.62072300
C	2.48640700	3.05000000	-1.38211300
C	-0.31678100	0.86332400	-3.41703000
C	-2.69287800	-1.09704700	-0.67591000
C	1.27611100	-1.13192300	3.46769900

C	-1.13759000	-2.99057000	0.73083900
C	0.10539100	-1.89418800	-3.01369400
C	3.31179700	0.63533800	-2.58711800
C	4.01680300	1.11016300	1.41399300
C	0.20024500	-1.98008500	3.02023200
C	3.37128000	0.56625600	2.58212000
C	3.99635800	1.15563000	-1.42512300
C	1.19074400	-1.03643300	-3.48551200
C	-1.15677700	-2.96676400	-0.71068400
C	-0.23931700	0.75463800	3.50916800
C	-2.62340500	-1.08937200	0.74040500
C	-1.40638400	0.00548500	-2.93397100
C	1.80202000	2.52701600	-2.54049800
C	2.49985100	2.99411800	1.45289600
C	-1.07117700	-1.43953600	2.67391700
C	2.19241700	1.15967200	3.11893100
C	3.49201300	2.28989900	-0.72345000
C	1.01468100	0.37420000	-3.53075800
C	-1.81883800	-1.93158000	-1.43111100
C	1.10336200	0.27566900	3.58026100
C	-1.75732800	-1.96196800	1.47694700
C	-1.15307200	-1.37868700	-2.63164500
C	2.11967300	1.24463900	-3.07716800
C	3.50328200	2.26300300	0.75364000
C	-2.70273000	2.40634800	0.09106100
C	-3.18456300	1.10425900	0.08476700
C	-3.29014600	0.23251600	-1.19504800
C	-4.76422300	0.08881100	-1.74492500
H	-5.05420100	1.08200400	-2.10835400

H	-4.70659400	-0.56856000	-2.62076400
C	-5.79653600	-0.42948100	-0.76848600
C	-6.51465000	0.45483600	0.05664500
C	-6.05760500	-1.80659100	-0.65331400
C	-7.46397500	-0.02023300	0.96765700
H	-6.32100300	1.52113100	-0.01567900
C	-7.00630800	-2.28609100	0.25636700
H	-5.50898300	-2.50406200	-1.27975200
C	-7.71392300	-1.39385600	1.07049300
H	-8.00619100	0.68041500	1.59613700
H	-7.19127500	-3.35392700	0.32979900
H	-8.45038000	-1.76461500	1.77741500
C	-2.35907900	0.79512500	-2.25416800

Total energy = –2937.6069 a.u.

Lowest frequency = 19.7 cm^{-1}

Geometry of 7-$PhCH_2C_{70}^-$

-1 1

C	-2.00180100	2.98629500	-1.19822300
C	-2.64850400	2.49569200	-0.00254800
C	-1.94345000	3.06131700	1.15628100
C	-0.86591400	3.89703900	0.66394400
C	2.84985200	-3.31347700	-1.11060800
C	3.95647100	-2.45799700	-0.69859500
C	3.98237600	-2.41848900	0.75863900
C	2.89409600	-3.24186700	1.25146300
C	2.18430300	-3.79307900	0.09492500

C	-1.85306800	2.12926100	-2.29848200
C	-3.10838700	1.17320400	0.03305500
C	-1.75061200	2.27020100	2.29124000
C	0.37124300	3.91219600	1.33922600
C	0.30671200	3.81340700	-1.51438700
C	2.09302200	-2.97944500	-2.23956600
C	4.25319000	-1.30403700	-1.43722400
C	4.30403400	-1.21589600	1.41572300
C	2.15508600	-2.83197900	2.36957500
C	0.79330000	-3.90897700	0.12039800
C	-0.60520500	2.09774800	-3.03364800
C	-2.25213200	0.90615200	2.34319700
C	0.56798600	3.10503900	2.52058100
C	1.57967500	3.82026800	-0.81419800
C	0.64448900	-3.10320800	-2.20610300
C	3.45095900	-0.95462300	-2.60001000
C	4.59386100	-0.01750400	0.63835400
C	2.49127200	-1.58043300	3.04638400
C	0.02309200	-3.48861800	1.29240400
C	2.39697400	-1.77409600	-2.99370900
C	0.01322500	-3.54795400	-1.04783400
C	0.71267100	-2.96821900	2.40644000
C	3.54973600	-0.79634200	2.57456000
C	4.57175300	-0.06236400	-0.75282400
C	-2.36031100	0.76893500	-2.24588500
C	0.45130100	2.91952100	-2.65330400
C	1.61216200	3.86445500	0.57690700
C	-0.47094300	2.28822600	2.98925100
C	-2.89153200	0.35248800	1.21930600

C	-0.34840700	0.72234500	-3.44957500
C	-1.29759600	0.10528500	3.05234900
C	1.92152500	2.57301100	2.49758500
C	2.50521800	2.95426400	-1.53029800
C	0.06602600	-2.00144800	-2.94034700
C	3.29379100	0.49076300	-2.63839300
C	4.05219100	1.13599800	1.33705800
C	1.27436900	-0.96537400	3.51108900
C	-1.22586200	-2.94411700	0.86721800
C	1.14414700	-1.17803800	-3.43495900
C	-1.22857100	-2.93686000	-0.60681600
C	0.17429700	-1.81288900	3.07990600
C	3.39241400	0.65062200	2.52327900
C	3.98350500	1.04099500	-1.49973100
C	-1.42042900	-0.09382500	-2.97761500
C	1.81254800	2.40331600	-2.66561800
C	2.57600800	3.05505700	1.30479000
C	-0.19827400	0.96123200	3.48057400
C	-2.70662900	-1.00210000	0.83973300
C	0.99136800	0.22546300	-3.56185600
C	-1.85785400	-1.94777100	-1.36339500
C	-1.08826400	-1.26246700	2.71413200
C	2.23175200	1.29310100	3.04546400
C	3.51392100	2.21602600	-0.84599500
C	-1.18770900	-1.43847600	-2.55209800
C	2.10764200	1.09587700	-3.14873700
C	3.54835200	2.26574400	0.62926500
C	1.12779500	0.45214300	3.55325900
C	-1.81625700	-1.83419100	1.55970600

C	-0.89317800	3.84584900	-0.79256000
C	-3.01117400	0.30938900	-1.11603600
C	-3.00446600	-1.17053300	-0.68306000
C	-4.36324200	-1.91866400	-0.99361300
H	-4.44917500	-1.98607200	-2.08541900
H	-4.24750200	-2.94129200	-0.61547500
C	-5.61118800	-1.28847600	-0.41715400
C	-6.36174000	-0.36322300	-1.16421600
C	-6.04844100	-1.60902400	0.88038900
C	-7.51560800	0.22326900	-0.63366000
H	-6.03363400	-0.10051000	-2.16595600
C	-7.20186400	-1.02454100	1.41462700
H	-5.47563700	-2.31591700	1.47286500
C	-7.94056200	-0.10666400	0.65874000
H	-8.08013400	0.93649900	-1.22732400
H	-7.52131400	-1.28407400	2.41974100
H	-8.83580800	0.34793400	1.07277000

Total energy = –2937.6095 a.u.

Lowest frequency = 21.9 cm^{-1}

Geometry of 21-$PhCH_2C_{70}^-$

-1 1

C	-3.32380500	-3.19136800	0.03201400
C	-2.52257600	-3.50671200	-1.14428200
C	-1.22707000	-3.99838700	-0.68618800
C	-1.23016700	-4.00187300	0.76903300
C	-0.47353000	4.24557900	-0.02350400

C	0.32874600	3.94772300	1.15809100
C	1.62924800	3.45964700	0.71314600
C	1.62278900	3.43576300	-0.74143200
C	0.32809500	3.92904000	-1.19947900
C	-4.16091200	-2.06782400	0.02175700
C	-2.59367100	-2.68441400	-2.27426000
C	-0.06763200	-3.64074800	-1.38098900
C	-0.05858400	-3.62168900	1.44586000
C	-2.60316500	-2.65343800	2.33426500
C	-1.84706200	3.96954200	-0.02343700
C	-0.28573600	3.39416300	2.28915900
C	2.24862600	2.40173500	1.39962800
C	2.24333100	2.38469700	-1.42500100
C	-0.27962300	3.34971600	-2.31902400
C	-4.23033700	-1.19625400	1.18348300
C	-0.14920700	-2.77607400	-2.53328600
C	1.15218400	-3.27591200	0.73142100
C	-1.38880800	-2.27119800	3.03966200
C	-2.47127100	3.36270100	-1.18877000
C	-1.70855700	3.09717500	2.27608400
C	1.59353700	1.82255800	2.56604300
C	2.90297100	1.29325200	-0.70306000
C	0.37138400	2.25259100	-3.01770600
C	-2.47570000	3.38306900	1.14916700
C	-1.70476100	3.05821300	-2.30957700
C	1.59963500	1.78046500	-2.56593100
C	2.91247600	1.32607100	0.69513300
C	0.36581800	2.30741100	3.00549200
C	-4.22559300	-1.21451000	-1.15435600

C	-3.46371000	-1.48203800	2.31070700
C	-0.15325900	-2.73698000	2.60057300
C	1.15524500	-3.25772700	-0.66854900
C	-1.38024600	-2.31280100	-2.98530200
C	-4.35556800	0.17855800	0.72446800
C	1.01870300	-1.89622100	-2.51950600
C	1.79518500	-2.16078900	1.43302600
C	-1.52173600	-0.88742400	3.47165900
C	-3.48836600	2.42646100	-0.73246700
C	-1.93470800	1.85968500	3.00920100
C	1.85285100	0.39632400	2.57147400
C	2.73888300	0.06189900	-1.43748200
C	-3.48931000	2.43761600	0.70738100
C	-1.92230300	1.80624300	-3.02064900
C	1.88444900	0.34573600	-2.53725100
C	2.65055700	0.07692600	1.41582800
C	-0.65556000	1.37232600	3.45462900
C	-4.35487400	0.16749900	-0.71561500
C	-2.80101300	-0.40084400	3.02610300
C	0.99277900	-1.84968000	2.58873400
C	1.84349500	-2.23693200	-1.41552700
C	-1.50911400	-0.94258800	-3.44312800
C	-3.79595000	1.26519000	1.45812100
C	-2.97753500	0.92084300	-2.65559500
C	-0.39170500	-0.02396800	3.56153100
C	-3.78608800	1.23949700	-1.46319500
C	-2.98323700	0.96250400	2.65192700
C	0.91269900	-0.52735900	3.10261800
C	-0.36341800	-0.08737600	-3.52576000

C	-2.52127500	-3.49029000	1.21354000
C	-3.45851900	-1.51491400	-2.27578100
C	-2.78644400	-0.44755300	-3.00371300
C	-0.64325200	1.31481900	-3.45937000
C	2.90069800	-1.31853600	-0.77626800
C	4.33951400	-1.95227800	-0.98042600
H	4.30698000	-2.95668600	-0.53871900
H	4.46310100	-2.07864700	-2.06283600
C	0.93802400	-0.58255700	-3.08346200
C	5.50653700	-1.17586100	-0.41522400
C	6.15576400	-0.19027700	-1.18151700
C	5.97230600	-1.41576800	0.89051500
C	7.23240800	0.53445200	-0.65982200
H	5.80567200	0.00964300	-2.18956000
C	7.04927700	-0.69374800	1.41542000
H	5.48157600	-2.17156200	1.49674000
C	7.68415800	0.28495800	0.64151100
H	7.71654800	1.29336300	-1.26793100
H	7.39126400	-0.89448100	2.42681800
H	8.52022200	0.84682400	1.04788100
C	2.56169300	-1.17581300	0.76875600

Total energy = –2937.5831 a.u.

Lowest frequency = 18.8 cm^{-1}

Geometry of **2**

0 1

C	2.58952800	-3.49234200	1.19536100

C	1.25538300	-3.98265600	0.87279200
C	1.13476800	-4.03164700	-0.58013600
C	2.38759300	-3.58390200	-1.15459400
C	3.28974900	-3.24277100	-0.06015800
C	-0.17846900	3.98336000	1.13322100
C	0.52929200	4.23594500	-0.11754700
C	-0.36610100	3.89102700	-1.21481100
C	-1.62224000	3.42249100	-0.63847300
C	-1.51009600	3.48633900	0.80474000
C	2.76409800	-2.61881200	2.27454600
C	0.16346900	-3.58400400	1.64691300
C	-0.07523200	-3.66555800	-1.19599100
C	2.36193100	-2.78876700	-2.30677400
C	4.12653600	-2.12842000	-0.17537600
C	0.51213500	3.44093900	2.22136700
C	1.89337900	3.93900400	-0.21683600
C	0.14526500	3.27457200	-2.35906500
C	-2.30706500	2.34599900	-1.22898400
C	-2.08057600	2.46682400	1.57555300
C	3.63549100	-1.46182800	2.14537100
C	0.35004000	-2.67719800	2.76839400
C	-1.19883600	-3.23657700	-0.38262900
C	1.10209400	-2.43771300	-2.93362000
C	4.09986400	-1.31112300	-1.37961900
C	-0.09154800	2.38779700	3.02466300
C	2.60307500	3.37423300	0.91982200
C	1.56375100	2.97004400	-2.45925100
C	-1.75778600	1.70305900	-2.40841200
C	-2.79626300	1.37467900	0.94346800

C	1.92732100	3.13077800	2.11107000
C	-1.35596300	1.91181900	2.70493200
C	-2.93676500	1.32914500	-0.42751100
C	-0.56938900	2.16478500	-2.96992200
C	2.42024600	3.29483000	-1.41035300
C	1.62309900	-2.20485800	3.07699100
C	4.30114400	-1.22266300	0.94750800
C	3.23521900	-1.63368700	-2.41695500
C	-0.08937500	-2.89417800	-2.41027900
C	-1.08788400	-3.21130200	1.00607200
C	3.04291700	-0.35267800	2.87789100
C	-0.78949300	-1.77764200	2.82728700
C	-1.94598900	-2.21941700	-1.07801600
C	1.21710000	-1.06084100	-3.43872300
C	4.28283800	0.08315300	-0.99511600
C	0.95496000	1.45410300	3.42294900
C	3.57072400	2.40590700	0.42589500
C	1.71401700	1.69898100	-3.14796500
C	-2.05632500	0.29449500	-2.37425300
C	-2.51271100	0.14933900	1.70486100
C	2.19435300	1.91131100	2.85998200
C	-1.63908500	0.48323200	2.78019500
C	0.38860200	1.20504100	-3.45448300
C	3.45339500	2.35532800	-1.01030900
C	1.80077400	-0.81196100	3.44875300
C	4.40461900	0.13610300	0.43469900
C	2.52154400	-0.57838200	-3.12664500
C	-1.67017400	-2.10999700	1.72765800
C	3.20440400	0.99238100	2.44673900

C	-0.65715600	-0.44014900	3.26846600
C	-2.57897400	-1.19481400	-0.40152000
C	0.09127700	-0.18543100	-3.45923300
C	3.67456600	1.14345100	-1.72663200
C	0.68760100	0.06561200	3.59709000
C	3.91511500	1.25030800	1.17943200
C	2.76456200	0.80433700	-2.83509800
C	-1.19031000	-0.63698600	-2.90901800
C	-2.43517300	-1.11739600	1.05545700
C	-1.40455200	-2.10749800	-2.52861100
H	-2.08157100	-2.58664700	-3.25306300
C	-3.06681100	0.01381900	-1.22058600
C	-4.52397200	-0.20923800	-1.78942200
H	-4.75576100	0.65351300	-2.42481600
H	-4.48267500	-1.08974700	-2.44119300
C	-5.60533500	-0.39026000	-0.74410000
C	-5.96108500	-1.67247600	-0.29040800
C	-6.27935000	0.72197100	-0.21015100
C	-6.95894600	-1.83899300	0.67562700
H	-5.45629300	-2.54302100	-0.69925100
C	-7.27777800	0.55852300	0.75578400
H	-6.02329000	1.71911900	-0.55653900
C	-7.61976700	-0.72319000	1.20236400
H	-7.22217900	-2.83679700	1.01239000
H	-7.78969800	1.42866400	1.15462300
H	-8.39612300	-0.85132000	1.94989100

Total energy = –2938.1227 a.u.

Lowest frequency = 20.3 cm^{-1}

Geometry of **4**

0 1

C	2.71512200	1.93756300	-1.19843100
C	2.27760700	2.81538700	-0.14295700
C	2.57033400	2.17597700	1.12790200
C	3.19607800	0.90321300	0.86122000
C	-4.52438300	-1.39542500	-1.21927000
C	-3.97346300	-2.59731300	-0.60205400
C	-4.05074600	-2.43324500	0.84564300
C	-4.65179200	-1.13368200	1.12057900
C	-4.94400200	-0.49322500	-0.15377900
C	1.94469200	1.81884100	-2.33896700
C	1.11354000	3.59051300	-0.28433300
C	1.68557400	2.33744000	2.20831100
C	2.85875600	-0.18371600	1.64590400
C	-3.93533300	-0.87714800	-2.37766500
C	-2.86071600	-3.22275900	-1.17200200
C	-3.01065300	-2.90340600	1.65419600
C	-4.18041000	-0.36486800	2.19210300
C	-4.75129300	0.88674900	-0.29759400
C	1.68613200	0.49768600	-2.94473100
C	0.32072500	3.46872200	-1.48090600
C	0.46820600	3.11876300	2.04667500
C	1.92140600	-0.03899900	2.74238200
C	2.67613700	-1.66686800	-0.31939900
C	-3.73209300	0.55660100	-2.51722200
C	-2.24939200	-2.67682900	-2.37461000

C	-1.85304600	-3.54801100	1.05477900
C	-3.09391700	-0.85630000	3.02284000
C	-4.25984400	1.67794300	0.81837100
C	-2.77388600	-1.52906900	-2.96150700
C	-4.12988200	1.41639100	-1.49945400
C	-3.98080600	1.06618900	2.03504000
C	-2.52196000	-2.09658600	2.76148500
C	-1.77997600	-3.70656200	-0.32611200
C	0.72372900	2.58726500	-2.48287800
C	2.20840700	-0.63661000	-2.37361200
C	2.59987300	-1.50516200	1.04155100
C	1.35448400	1.20150100	3.02972500
C	0.18916700	3.73065300	0.83062400
C	0.32539500	0.49619500	-3.45125700
C	-1.08729900	3.55220600	-1.11822700
C	-0.59938600	2.46987600	2.79177900
C	1.11340500	-1.24085300	2.83399200
C	1.67166200	-2.44349600	-0.99720700
C	-2.46664600	0.78040000	-3.20082700
C	-0.80874400	-2.84096200	-2.27363800
C	-0.66874800	-3.15783400	1.80312400
C	-2.24660200	0.26967700	3.39041100
C	-3.36337600	2.70391900	0.30189600
C	-1.87870200	-0.50465000	-3.47570600
C	-3.28159000	2.53957000	-1.12582400
C	-2.79402800	1.45543500	2.78536800
C	-1.07913700	-2.26251700	2.85338000
C	-0.51990700	-3.47494600	-1.01200200
C	-0.26338100	1.77833900	-3.17323800

C	1.38417200	-1.81147100	-2.25732900
C	1.52594200	-2.13614200	1.78715900
C	-0.05273100	1.28344100	3.39550700
C	-1.16850700	3.71754700	0.30897100
C	-0.46657400	-0.68697000	-3.47093200
C	-2.08444100	2.83447000	-1.83733600
C	-1.95330900	2.51696100	2.34909200
C	-0.23633500	-1.20171100	3.28945800
C	0.66933900	-3.17571600	-0.29165400
C	-1.65766000	1.91530400	-2.91139000
C	0.08493900	-1.89322700	-2.84450600
C	0.59545200	-3.01585200	1.16435500
C	-0.84373000	0.11354900	3.57575700
C	-2.24959600	3.16663400	1.05638200
C	3.59843900	0.80414200	-0.62761100
C	5.11812500	1.16433200	-0.87000500
H	5.25087100	1.27627200	-1.95317800
H	5.28649700	2.15347700	-0.42839200
C	6.13136100	0.17313700	-0.33433100
C	6.44615200	0.12365100	1.03661800
C	6.79405000	-0.71201700	-1.20388200
C	7.38191700	-0.79402400	1.52305700
H	5.95968600	0.80941400	1.72281700
C	7.73031500	-1.63306400	-0.71915100
H	6.58987800	-0.66609300	-2.27073200
C	8.02405800	-1.67862700	0.64734700
H	7.61319800	-0.81587100	2.58335900
H	8.23183800	-2.30574100	-1.40777500
H	8.75091900	-2.38976200	1.02647400

C	3.27251900	-0.62496800	-1.27058100
H	4.22198800	-1.00983800	-1.66575900

Total energy = –2938.1340 a.u.

Lowest frequency = 20.5 cm^{-1}

Geometry of **5**

0 1

C	0.50579500	4.23635600	0.04983500
C	-0.34255500	3.93131400	-1.09637100
C	-1.60814300	3.43019400	-0.59866200
C	-1.56277300	3.43837100	0.84926400
C	-0.25206400	3.93042800	1.25860000
C	3.30628600	-3.22237800	-0.08450800
C	2.54793500	-3.52848500	1.12399500
C	1.23220500	-4.01065500	0.72145100
C	1.17566500	-3.99347800	-0.73556000
C	2.46010500	-3.51586800	-1.23515600
C	1.87178600	3.94113300	-0.00461100
C	0.21609200	3.34539900	-2.23598100
C	-2.26017800	2.37387600	-1.27376900
C	-2.15798200	2.38505600	1.54869900
C	0.39414400	3.34419400	2.35148000
C	4.14957100	-2.10620600	-0.11095100
C	2.66958100	-2.70414500	2.24766800
C	0.10332400	-3.65219400	1.46430800
C	-0.00630600	-3.60570100	-1.37902900
C	2.50185500	-2.68436400	-2.35848900

C	2.53663900	3.33444100	1.13570300
C	1.63736200	3.05014400	-2.28862800
C	-1.69505600	1.81857400	-2.47207100
C	-2.83684000	1.31913000	0.83955300
C	-0.23842400	2.25529500	3.08311600
C	4.18491400	-1.24117200	-1.27953800
C	3.54205000	-1.54116700	2.21037700
C	0.23664300	-2.79263400	2.63012600
C	-1.17377300	-3.22798900	-0.60428100
C	1.26978600	-2.29509500	-3.02653500
C	4.26503200	-1.24908900	1.05831700
C	3.37942100	-1.52422200	-2.37876600
C	0.04177900	-2.74045000	-2.54230700
C	-1.12252500	-3.25903500	0.78710900
C	1.49148900	-2.32956600	3.01452600
C	2.44802000	3.34121300	-1.19982900
C	1.81374300	3.04204200	2.28797800
C	-1.48460400	1.78802400	2.68901600
C	-2.91520700	1.32542800	-0.53810800
C	-0.47443700	2.27456500	-2.92548100
C	3.53038200	2.38948900	0.64495600
C	1.82356000	1.80836800	-3.02868400
C	-2.59240800	0.06735200	1.56689000
C	0.79409200	1.30895200	3.48751200
C	4.33568800	0.13337400	-0.83133200
C	2.91149100	-0.46698100	2.96128200
C	-0.90939700	-1.89953400	2.67774800
C	-1.87873500	-2.15903200	-1.28748200
C	1.39181300	-0.92541800	-3.46205600

C	4.38726300	0.12908100	0.60988700
C	2.69833900	-0.44310100	-3.07210900
C	-1.73996300	-2.18808700	1.52947700
C	1.64699900	-0.95299400	3.45526900
C	3.47723200	2.39322200	-0.79083000
C	2.05512700	1.79330700	2.99748900
C	-1.76565600	0.35807900	2.69294300
C	0.53697300	1.33129600	-3.42133900
C	3.85377300	1.20604400	1.37079800
C	2.89381300	0.91110300	-2.71033300
C	-1.03450700	-0.56460000	-3.03041800
C	-2.48463700	-1.16970000	0.86918000
C	0.52566800	-0.08567900	3.59140300
C	3.74789400	1.21622200	-1.54534000
C	3.08656900	0.89613800	2.59393300
C	-0.80347100	-0.58235200	3.18342200
C	-2.56905900	-1.17684800	-0.59357600
C	0.25862600	-0.06380100	-3.50240000
C	-3.06688600	0.04970700	-1.37250400
C	-1.10332700	-1.85072700	-2.52329700
C	-4.55642500	-0.17722900	-1.85345300
H	-4.83597200	0.70470200	-2.44426700
H	-4.53684000	-1.03523400	-2.53696000
C	-2.18338300	0.39361100	-2.71003900
H	-2.88780000	0.36745900	-3.55472700
C	-5.58523400	-0.41042700	-0.76730200
C	-6.25205300	0.67048100	-0.16420200
C	-5.90582900	-1.71420400	-0.34943800
C	-7.20728300	0.45567900	0.83503400

H	-6.02440600	1.68375000	-0.48202200
C	-6.86080500	-1.93210200	0.64883400
H	-5.40662300	-2.56088300	-0.81172500
C	-7.51345400	-0.84686800	1.24535400
H	-7.71351600	1.30237400	1.28787500
H	-7.09727300	-2.94575500	0.95682900
H	-8.25647600	-1.01503300	2.01838900

Total energy = –2938.1173 a.u.

Lowest frequency = 22.3 cm^{-1}

Geometry of **6**

0 1

C	1.03366100	3.84424000	0.58547900
C	2.10825400	2.96677400	1.02929300
C	2.73068600	2.38163200	-0.15487500
C	2.04898100	2.89665300	-1.32315600
C	0.99432400	3.79909900	-0.87121200
C	-4.05715800	-2.28390500	0.90326800
C	-4.10158100	-2.32476800	-0.55462100
C	-3.05079200	-3.22762500	-1.00986100
C	-2.35685000	-3.74369900	0.16306000
C	-2.97752800	-3.16090600	1.34414800
C	-0.16285300	3.90052800	1.31327700
C	1.94191600	2.19155300	2.17910500
C	3.15312100	1.04417300	-0.14044800
C	1.81506800	2.03685000	-2.40186600
C	-0.23917000	3.80959000	-1.53095900

C	-4.28618800	-1.07668600	1.57020800
C	-4.37664900	-1.15552700	-1.27241900
C	-2.31523100	-2.91373800	-2.15960600
C	-0.96903200	-3.92590800	0.12382500
C	-2.17787000	-2.78151200	2.42818000
C	-1.43878000	3.90593300	0.61879300
C	0.69888500	2.25255300	2.93252100
C	2.95900700	0.24098900	1.05348800
C	2.27616900	0.65983100	-2.36894500
C	-0.47328600	2.92432300	-2.66037600
C	-3.45183400	-0.69077100	2.69785000
C	-4.60979000	0.09724300	-0.57220100
C	-2.60257100	-1.69193700	-2.89418900
C	-0.21058000	-3.60381600	-1.07566600
C	-0.73689500	-2.95482000	2.36394100
C	-4.56697300	0.13695800	0.81725100
C	-2.42043900	-1.52247600	3.11389400
C	-0.14802900	-3.51294200	1.24266400
C	-0.87548700	-3.10173100	-2.18635100
C	-3.60957900	-0.83505400	-2.46667100
C	-0.33251100	3.08798100	2.50710900
C	-1.47709000	3.86353400	-0.77116100
C	0.53027100	2.05574700	-3.07871900
C	2.97111800	0.17902200	-1.28021300
C	2.37991600	0.80613700	2.19252700
C	-2.39203000	3.12230900	1.39173900
C	0.39337000	0.92095900	3.42201800
C	1.25741800	-0.16820900	-3.04031600
C	-1.85182300	2.46230600	-2.60891400

C	-3.24472400	0.75154700	2.64698100
C	-4.01516100	1.17888100	-1.34466700
C	-1.34857300	-1.14081200	-3.37974900
C	1.07869200	-3.04834300	-0.67893100
C	-0.10522000	-1.81849500	3.03155100
C	-3.92955200	1.25677800	1.49043800
C	-1.13702100	-0.94656500	3.49743000
C	-0.28176700	-1.99498200	-2.94057100
C	-3.39996200	0.60496700	-2.51113600
C	-1.70609400	2.61687000	2.55562200
C	-2.46891800	3.03745500	-1.44321200
C	0.19649100	0.70135500	-3.47551100
C	1.43804000	0.03016400	2.95484300
C	-3.42396800	2.37662600	0.76110000
C	-0.94274300	0.46928500	3.56019300
C	1.80916900	-1.89908800	1.41825800
C	1.00419100	-1.49021800	-2.65358200
C	-2.21965600	1.16867100	-3.07713100
C	-2.03811900	1.34928700	3.11384000
C	-3.46762400	2.33274600	-0.71208900
C	-1.15435100	0.25824900	-3.52857400
C	1.16097100	-1.31948400	2.61137100
C	1.10755800	-2.96388000	0.71119000
C	2.67971600	-1.11105900	0.67043200
C	2.98502800	-1.29878000	-0.84027100
C	1.92742800	-2.22799900	-1.63767300
H	2.55154600	-2.92092700	-2.22445200
C	4.40006200	-1.97257800	-1.06182700
H	4.55646500	-2.01918200	-2.14718500

H	4.31341500	-3.00612700	-0.70315900
C	5.58971300	-1.30361700	-0.40739400
C	6.31106600	-0.30398600	-1.08333900
C	6.00689900	-1.67684900	0.88192400
C	7.41436900	0.31278400	-0.48407300
H	6.00741300	-0.00995000	-2.08410900
C	7.11003200	-1.06239600	1.48399800
H	5.46496500	-2.45298000	1.41476300
C	7.81611900	-0.06416400	0.80264300
H	7.96022000	1.08191200	-1.02143900
H	7.41870500	-1.36431900	2.47988000
H	8.67332700	0.41203300	1.26781200

Total energy = –2938.1031 a.u.

Lowest frequency = 23.5 cm^{-1}

Geometry of **7**

0 1

C	2.65706500	2.09204000	-1.20554100
C	2.22071100	2.91708000	-0.11082500
C	2.55786000	2.24143700	1.13259200
C	3.22440200	0.99597700	0.82659900
C	-4.49124900	-1.45812400	-1.18773600
C	-3.88973100	-2.65836500	-0.62143600
C	-3.93813000	-2.54445500	0.83179900
C	-4.57193200	-1.27454600	1.16505000
C	-4.91100700	-0.60143000	-0.08216600
C	1.85635100	1.98759100	-2.33128800

C	1.02626700	3.65711000	-0.20286300
C	1.68826700	2.34165200	2.23058200
C	2.95247500	-0.12019600	1.59082000
C	-3.94231800	-0.88520200	-2.33999900
C	-2.77026500	-3.23153000	-1.23639100
C	-2.86307200	-3.00644600	1.59964700
C	-4.10054700	-0.52681300	2.25033900
C	-4.76041200	0.78525400	-0.18319800
C	1.61479200	0.67934200	-2.97302900
C	0.20872400	3.55453200	-1.38796400
C	0.44494800	3.09112000	2.12093400
C	2.00588800	-0.03837300	2.67125200
C	2.73025000	-1.48268700	-0.46416400
C	-3.78271900	0.55696900	-2.43413600
C	-2.20644700	-2.63093300	-2.43377800
C	-1.69892600	-3.58901300	0.95249600
C	-2.98142800	-1.01253700	3.04186500
C	-4.26866000	1.55610500	0.94670800
C	-2.77852100	-1.48427300	-2.97435800
C	-4.17941400	1.37184700	-1.38187900
C	-3.94591500	0.91428400	2.13702900
C	-2.37852800	-2.22445800	2.72525600
C	-1.65390000	-3.70272500	-0.43194700
C	0.61450800	2.72189700	-2.42666600
C	2.17471900	-0.45531800	-2.43446900
C	2.92459800	-1.55165600	1.02674400
C	1.40777200	1.17130200	3.01792700
C	0.12260800	3.73295600	0.93175700
C	0.24926300	0.65176200	-3.47154500

C	-1.19363700	3.58435200	-0.99371400
C	-0.58716800	2.38757300	2.86590100
C	1.23199100	-1.27108800	2.73372000
C	1.73252000	-2.31956700	-1.14560900
C	-2.53677400	0.83940400	-3.13677900
C	-0.75701800	-2.75820100	-2.37780200
C	-0.50878700	-3.18446300	1.68570800
C	-2.15997300	0.12490700	3.42764700
C	-3.41225700	2.62173000	0.44454300
C	-1.92164300	-0.41713800	-3.47419200
C	-3.35685800	2.50765600	-0.98909900
C	-2.75505000	1.31443300	2.87488000
C	-0.92827300	-2.34644100	2.78096800
C	-0.41546500	-3.41412200	-1.13968000
C	-0.36686600	1.90266600	-3.12757500
C	1.40118200	-1.68216000	-2.38131000
C	1.66083000	-2.12850200	1.69248100
C	0.00494000	1.19983800	3.41350900
C	-1.24717300	3.69762200	0.43857200
C	-0.50646300	-0.55806000	-3.51356600
C	-2.18501900	2.86048600	-1.71502000
C	-1.95389800	2.41116900	2.45490200
C	-0.11378400	-1.28017800	3.22745900
C	0.78724300	-3.10506500	-0.44233800
C	-1.75712000	1.98963200	-2.82841500
C	0.09586900	-1.77444900	-2.94418000
C	0.74322900	-2.99258800	1.04106100
C	-0.74906700	0.00342700	3.57266700
C	-2.29509800	3.09255200	1.19092400

C	3.55695500	0.93416200	-0.68811600
C	5.07321700	1.19207300	-1.02957800
H	5.15798500	1.22722700	-2.12204200
H	5.32722600	2.18930100	-0.65212200
C	6.02619500	0.16131100	-0.46269300
C	6.59777900	0.33649700	0.81009400
C	6.35062700	-0.99701800	-1.19081700
C	7.46643200	-0.62167800	1.34375300
H	6.36404000	1.22979800	1.38215900
C	7.21866500	-1.95721300	-0.65966400
H	5.92383700	-1.14393100	-2.17856600
C	7.77781600	-1.77306200	0.61059900
H	7.90244400	-0.46704000	2.32578700
H	7.46125900	-2.84329900	-1.23795000
H	8.45453100	-2.51544500	1.02168900
C	3.01161800	-0.37939200	-1.22653500
H	3.82027600	-2.13028600	1.30071200

Total energy = –2938.1212 a.u.

Lowest frequency = 23.6 cm^{-1}