

Article

Interaction of Several Toxic Heterocarbonyl Gases with Polypyrrole as a Potential Gas Sensor

Francisco C. Franco Jr

Chemistry Department, De La Salle University, 2401 Taft Avenue, 0922 Manila, Philippines;
francisco.franco@dlsu.edu.ph; Tel.: +63-2-85360230

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Table S1. Cartesian coordinates, lowest vibrational frequencies, and total energies of 9Py and the 9Py-HC complexes.

9Py							
H	11.78619600	0.50162500	-2.61683000	H	-6.92189500	-0.49355800	-1.45844600
C	11.11681600	0.53514500	-1.76852800	C	-11.11681500	0.53515000	-1.76853000
C	9.85449100	-0.10901600	-1.66422200	H	-11.78619300	0.50163200	-2.61683300
H	13.15610000	2.66788500	-1.97470500	N	-7.02162600	-0.63973800	-0.46606400
H	9.38302100	-0.72438800	-2.41769100	N	-3.55529900	-1.31400000	0.63377300
N	13.32228600	2.61277700	-0.98232900	C	0.71014700	-1.79104300	1.82396800
C	14.31521400	3.28027100	-0.30142500	H	8.48984600	-0.30421300	2.43819500
H	4.98658000	-2.15400600	-2.18564400	H	3.50383100	-0.84558200	1.52489900
C	11.38122800	1.15254700	-0.55079000	C	-5.98542100	-0.99385800	0.37589500
C	4.31795500	-1.90988600	-1.37202300	C	-0.71014800	-1.79104400	1.82396800
C	12.50577200	1.93814800	-0.09708500	C	-9.36412800	0.12227200	-0.38323500
C	9.36412800	0.12227100	-0.38323400	H	5.92069600	-1.14024000	2.57384300
H	6.92189700	-0.49356200	-1.45844400	C	-8.14259800	-0.29214400	0.26201500
C	2.91553500	-2.13205800	-1.33640200	C	-11.38122700	1.15254800	-0.55079100
H	2.31564200	-2.57723900	-2.11780600	H	-13.15610000	2.66789000	-1.97470300
N	7.02162600	-0.63973900	-0.46606200	H	1.35252400	-1.86475800	2.69031500
N	10.30886500	0.88423000	0.27613800	N	-13.32228500	2.61278000	-0.98232700
C	14.14060400	3.02935200	1.04539200	C	-6.46458000	-0.87859200	1.67696200
C	8.14259800	-0.29214300	0.26201700	H	-3.50383200	-0.84558500	1.52489800
C	4.69883000	-1.39577400	-0.13648400	N	-10.30886600	0.88422800	0.27613800
H	-2.31564000	-2.57723600	-2.11780800	C	-12.50577200	1.93814800	-0.09708400
C	13.00292700	2.18343900	1.17826000	C	-7.81363200	-0.43977600	1.60574300
C	5.98542100	-0.99385700	0.37589600	H	-1.35252500	-1.86475900	2.69031400
C	-2.91553400	-2.13205500	-1.33640400	C	-14.31521400	3.28027100	-0.30142100
C	2.45618500	-1.75107200	-0.07953100	H	-5.92069800	-1.14024600	2.57384100
H	0.00000000	-1.59047100	-1.28146300	C	-13.00292800	2.18343500	1.17826100
C	-4.31795400	-1.90988300	-1.37202600	H	-10.16265700	1.31951400	1.17359900
H	-4.98657900	-2.15400200	-2.18564700	C	-14.14060500	3.02934800	1.04539500
N	0.00000000	-1.75299100	-0.28660600	H	-8.48984900	-0.30422100	2.43819300
N	3.55529800	-1.31399900	0.63377400	H	-12.61696400	1.76140900	2.09572600
C	7.81363100	-0.43977100	1.60574500	H	-14.76673500	3.40052900	1.84402700
C	1.13565200	-1.76292600	0.49955100	H	15.05186400	3.87059300	-0.82463300
H	14.76673300	3.40053600	1.84402300	H	-15.05186400	3.87059400	-0.82462900
H	10.16265600	1.31951800	1.17359800	Low frequencies — 4.5875 10.3614 12.9660			
C	6.46457800	-0.87858800	1.67696400	SCF energy — -1882.33290635 A.U.			
C	-2.45618500	-1.75107100	-0.07953200				
H	-9.38301900	-0.72438000	-2.41769600				
C	-1.13565200	-1.76292600	0.49955100				
H	12.61696200	1.76141500	2.09572600				
C	-9.85448900	-0.10901100	-1.66422500				
C	-4.69883000	-1.39577400	-0.13648600				

9Py-CCI			
H	11.85198200	1.13964900	-2.43107300
C	11.23075400	0.98402600	-1.56004600
C	9.99497100	0.28351600	-1.51956900



H	13.19252600	3.19513000	-1.45042400
H	9.49912700	-0.19362600	-2.35331000
N	13.41674100	2.95659500	-0.49738500
C	14.42750700	3.51887900	0.24921900
H	5.16484300	-1.80220100	-2.18534600
C	11.54595500	1.36600100	-0.26058600
C	4.53669900	-1.74860200	-1.30715400
C	12.67172500	2.09274000	0.27990600
C	9.57137000	0.24559200	-0.19516900
H	7.08941700	-0.24383700	-1.24531900
C	3.14571700	-2.02675800	-1.24678500
H	2.51210000	-2.32169700	-2.07123700
N	7.24970300	-0.57466300	-0.30669900
N	10.52996300	0.90268900	0.55125700
C	14.33729700	3.00676600	1.52865000
C	8.40023800	-0.33148600	0.41777400
C	4.97161100	-1.46845700	-0.01525200
H	-2.13251300	-3.06889200	-1.72276400
C	13.23365400	2.10725500	1.55186500
C	6.27317700	-1.12406800	0.50098100
C	-2.68114000	-2.57882300	-0.93122300
C	2.74685900	-1.91412200	0.08122000
H	0.22452800	-1.69857700	-0.97070200
C	-4.07161300	-2.28325300	-0.91554700
H	-4.78410800	-2.50700200	-1.69697900
N	0.29069600	-2.04243500	-0.02251300
N	3.87115300	-1.58111400	0.81153700
C	8.15227500	-0.74805300	1.72179900
C	1.45980600	-2.08454300	0.70826000
H	14.99714800	3.24149000	2.35153800
H	10.42216100	1.15182100	1.52212200
C	6.82208000	-1.24375900	1.77389800
C	-2.14995700	-2.18821800	0.29358500
H	-9.07463400	-0.79301400	-1.82551000
C	-0.80069100	-2.21283700	0.80736400
H	12.91293000	1.50169900	2.38807200
C	-9.47498400	-0.12057500	-1.07968700
C	-4.37225100	-1.71564000	0.31825900
H	-6.57297800	-0.70814000	-0.95687900
C	-10.69194700	0.60805500	-1.16578500
H	-11.39128000	0.59417200	-1.99010900
N	-6.64758700	-0.81355500	0.04284500
N	-3.19474900	-1.67961800	1.03997000
C	1.10484900	-2.30787600	2.03628100
H	8.87078900	-0.75017200	2.52950700
H	3.85876100	-1.30162200	1.77982800
C	-5.60932600	-1.21243300	0.86196600
C	-0.31186600	-2.38505600	2.09820600
C	-8.92548700	0.11715200	0.17585100
H	6.33757400	-1.69464700	2.62864900
C	-7.71425300	-0.36204700	0.79505100
C	-10.86985700	1.28255300	0.03731700
H	-12.58437900	2.87191800	-1.38056200
H	1.79196700	-2.45764600	2.85744900
N	-12.71825100	2.86193800	-0.38184100
C	-6.03148100	-1.01929500	2.17320000
H	-3.07471200	-1.18566100	1.91087100
N	-9.79080900	0.96602800	0.83799800
C	-11.92006100	2.16069000	0.49941200

C	-7.34826700	-0.48763500	2.13142000
H	-0.90920700	-2.60834100	2.97120500
C	-13.63740100	3.62033700	0.30733400
H	-5.47476300	-1.28800300	3.06006200
C	-12.35339000	2.48272100	1.78094900
H	-9.58424700	1.41815500	1.71503900
C	-13.43321900	3.40234700	1.65573700
H	-7.98269100	-0.27601500	2.98071100
H	-11.96575100	2.06487200	2.69962200
H	-14.00327300	3.84324400	2.46087700
H	15.11596900	4.22715600	-0.18580200
H	-14.34918300	4.24378100	-0.21185400
C	-1.74460800	0.06209900	-2.39356200
O	-0.68907400	-0.46922100	-2.51649600
Cl	-2.99663900	0.00769000	-3.62575900
Cl	-2.20347900	1.02322500	-1.00616700

Low frequencies — 4.3778 8.3966 10.5667
SCF energy — -2916.07499409 A.U.

9Py-CF			
H	-11.83609300	0.88713500	2.50609600
C	-11.19784400	0.80682300	1.63718100
C	-9.94886300	0.13255000	1.56743300
H	-13.19818400	2.98571900	1.65530000
H	-9.45820800	-0.39614700	2.37266100
N	-13.40208500	2.81435500	0.68343900
C	-14.41051700	3.41277300	-0.03779300
H	-5.09250600	-1.91297900	2.16461600
C	-11.49853900	1.27805500	0.36383800
C	-4.45104000	-1.78325300	1.30419400
C	-12.62840700	2.02326600	-0.14182900
C	-9.50286600	0.19955800	0.25157100
H	-7.03037500	-0.32364600	1.30734300
C	-3.05411600	-2.03083800	1.24861800
H	-2.42891500	-2.37504300	2.06031800
N	-7.16882200	-0.58702000	0.34421400
N	-10.46097600	0.89328100	-0.46160500
C	-14.28960100	2.99821100	-1.34961500
C	-8.31127600	-0.31053200	-0.38102800
C	-4.86979800	-1.41678900	0.02863200
H	2.23777200	-2.98485600	1.74797400
C	-13.16929700	2.12200500	-1.41914100
C	-6.16890200	-1.05811700	-0.48408700
C	2.79259600	-2.44840700	0.99146800
C	-2.63554200	-1.81350400	-0.06014600
H	-0.13497300	-1.62250200	1.04679800
C	4.18939800	-2.17828100	0.99152500
H	4.89691600	-2.45937500	1.75898200
N	-0.17873500	-1.90000300	0.07588000
N	-3.75389700	-1.44835300	-0.78430200
C	-8.03386200	-0.62497500	-1.70757200
C	-1.33555400	-1.91502700	-0.67537400
H	-14.93990400	3.28169900	-2.16471000
H	-10.34172500	1.21528400	-1.40942700
C	-6.69409300	-1.09255700	-1.77206000
C	2.27089100	-1.98741100	-0.21442800
H	9.24984200	-0.90947800	1.94058100
C	0.92825500	-1.99248700	-0.74583200

H	-12.82361000	1.58548500	-2.29175400
C	9.66745600	-0.21079400	1.22914100
C	4.50225600	-1.55455000	-0.21163500
H	6.74626100	-0.69036500	1.10112900
C	10.90948400	0.46992100	1.34377800
H	11.61412500	0.38633600	2.15940900
N	6.80844800	-0.74145000	0.09630700
N	3.32596400	-1.45739600	-0.93011900
C	-0.95629800	-2.04085700	-2.00943800
H	-8.73852200	-0.57951300	-2.52612900
H	-3.73069200	-1.09709600	-1.72874600
C	5.75169800	-1.05949800	-0.73453200
C	0.46212100	-2.08651700	-2.05319600
C	9.11694500	0.11509000	-0.00597800
H	-6.18714000	-1.47042300	-2.64891200
C	7.88536200	-0.28754200	-0.63946800
C	11.10147400	1.20376500	0.17813100
H	12.87919100	2.65360900	1.66582800
H	-1.62782400	-2.14766200	-2.84994100
N	13.00576900	2.69413300	0.66692300
C	6.17215100	-0.81082900	-2.03692700
H	3.21777900	-0.91899800	-1.77595700
N	10.00615500	0.96925700	-0.62855500
C	12.17784600	2.07006800	-0.24442100
C	7.50671400	-0.32818300	-1.97763500
H	1.07639800	-2.23920700	-2.92963000
C	13.94542700	3.45796200	0.01232000
H	5.60083900	-1.01129700	-2.93250900
C	12.61290700	2.44755500	-1.51012800
H	9.80826900	1.47690700	-1.47675800
C	13.72440000	3.32186600	-1.34416600
H	8.14257300	-0.09275600	-2.81952200
H	12.20473400	2.09445700	-2.44689800
H	14.30351000	3.78709200	-2.12889100
H	-15.11908700	4.07502900	0.43572900
H	14.68175000	4.02739200	0.55862300
C	1.86323100	0.04779000	2.44651100
O	0.81757600	-0.46855100	2.65090900
F	2.90698300	0.02092900	3.25826200
F	2.16737800	0.80219400	1.40600300

Low frequencies — 4.4596 9.1164 10.8990
SCF energy — -2195.37468765 A.U.

9Py-CH			
H	-11.85076400	0.01628000	2.70888100
C	-11.22136700	0.17179200	1.84370000
C	-9.91187200	-0.34502700	1.64944500
H	-13.43389200	2.08529100	2.27695300
H	-9.35781400	-0.96721200	2.33832100
N	-13.63347600	2.08771700	1.28923100
C	-14.70842900	2.70851600	0.69386600
H	-4.86308800	-1.93291600	1.87253000
C	-11.58811800	0.84782100	0.68513800
C	-4.25332300	-1.59691200	1.04549900
C	-12.79543700	1.55723000	0.32915700
C	-9.49551100	0.02127900	0.37371800
H	-6.96633600	-0.44314800	1.31735800
C	-2.84160600	-1.69976300	0.94403900

H	-2.17053500	-2.09754700	1.69195900
N	-7.09277800	-0.52660200	0.32081700
N	-10.52982000	0.73874600	-0.19480800
C	-14.56528000	2.57329500	-0.67307600
C	-8.26892800	-0.23265500	-0.34126000
C	-4.72800700	-1.04395500	-0.14036700
H	2.34875200	-3.07612700	0.86861100
C	-13.36250800	1.84775000	-0.90693500
C	-6.06411300	-0.72601700	-0.57907500
C	2.93137600	-2.33976800	0.33441200
C	-2.46840400	-1.21056800	-0.30487100
H	0.02624100	-1.69161500	0.71724900
C	4.34178100	-2.17059700	0.38692800
H	5.03669900	-2.75946100	0.96948800
N	-0.01732500	-1.41618900	-0.26025700
N	-3.62866600	-0.82151700	-0.94554700
C	-7.98283400	-0.25584800	-1.70244400
C	-1.17425900	-1.07202900	-0.92495900
H	-15.25314300	2.94223300	-1.42033100
H	-10.45869400	1.24833000	-1.06170200
C	-6.60430500	-0.56476100	-1.85136100
C	2.42832200	-1.43647900	-0.59809600
H	9.51749000	-1.75865400	1.45719000
C	1.08469700	-1.17045100	-1.05447500
H	-12.97679800	1.53093400	-1.86592300
C	9.97842600	-0.86797800	1.05349700
C	4.68510600	-1.16676600	-0.51375400
H	7.02740600	-1.05602800	0.90568000
C	11.27773800	-0.37847100	1.35610800
H	11.99052800	-0.82676700	2.03415800
N	7.05915000	-0.70366100	-0.03804300
N	3.51017500	-0.73923600	-1.10159900
C	-0.80008500	-0.60301600	-2.18337900
H	-8.70162900	-0.12523000	-2.49929000
H	-3.66473100	-0.35003300	-1.83509000
C	5.96043600	-0.59517000	-0.86822700
C	0.61481200	-0.66339700	-2.26355900
C	9.43103400	-0.04382700	0.07566200
H	-6.07718100	-0.71361000	-2.78341200
C	8.15528200	-0.07539100	-0.59632700
C	11.50736700	0.73869400	0.56037000
H	13.44257900	1.34975200	2.39273600
H	-1.46933400	-0.27444700	-2.96638300
N	13.54794500	1.77271300	1.48419400
C	6.37234400	0.11524900	-1.99147200
H	3.43353100	0.06454800	-1.70527600
N	10.37768200	0.91999000	-0.21206200
C	12.64624000	1.62094900	0.45008600
C	7.74454600	0.44024900	-1.82137500
H	1.22218500	-0.41732200	-3.12345000
C	14.53634700	2.66230800	1.12827100
H	5.76667700	0.32505200	-2.86199800
C	13.08312300	2.43472300	-0.58950200
H	10.20662800	1.73246000	-0.78382900
C	14.27188700	3.08917700	-0.15828300
H	8.37916300	0.94250400	-2.53799400
H	12.62296000	2.51082200	-1.56483800
H	14.87143600	3.78290600	-0.73002100
H	-15.47383300	3.18866000	1.28420700



H	15.33346100	2.91447900	1.81083600
C	1.32207100	-0.80097200	2.78442500
O	0.45500800	-1.64179200	2.65110300
H	1.80634600	-0.62935200	3.76290800
H	1.66413400	-0.17944200	1.93901000

Low frequencies — 3.4476 8.2106 11.2868

SCF energy — -1996.85911232 A.U.

9Py-CS			
H	11.83125000	1.00903700	-2.49989800
C	11.18766900	0.87810000	-1.64113900
C	9.94547500	0.18840700	-1.61524300
H	13.16414000	3.07665600	-1.53289000
H	9.46613500	-0.30365100	-2.44996700
N	13.36319700	2.85769400	-0.56962600
C	14.36015400	3.42872300	0.18879700
H	5.11745600	-1.88427900	-2.35003400
C	11.47419800	1.28719200	-0.34326500
C	4.46782000	-1.80099400	-1.49000800
C	12.59247000	2.01723700	0.20823000
C	9.48935700	0.18404100	-0.30115300
H	7.03033600	-0.31129400	-1.40101100
C	3.07301900	-2.06510000	-1.45736800
H	2.45886300	-2.38156100	-2.28862400
N	7.16474400	-0.62143500	-0.45132900
N	10.43488900	0.85050100	0.45359200
C	14.23472500	2.94608400	1.47670000
C	8.29886800	-0.36983800	0.29567000
C	4.87280200	-1.49083700	-0.19533100
H	-2.18668200	-2.83328900	-2.10816700
C	13.12351300	2.05583800	1.49289700
C	6.16413100	-1.14409100	0.34459300
C	-2.76283800	-2.41722800	-1.29400800
C	2.64206400	-1.91369700	-0.14327800
H	0.14887200	-1.65297900	-1.24905900
C	-4.16058100	-2.16675700	-1.28432000
H	-4.85277800	-2.35574500	-2.09283300
N	0.18528500	-1.99174100	-0.29887400
N	3.75098900	-1.57178400	0.60612100
C	8.01540200	-0.75355300	1.60258400
C	1.33885100	-2.05706500	0.45640100
H	14.87635400	3.19408000	2.31002900
H	10.30565100	1.12255500	1.41564500
C	6.68035700	-1.23771400	1.63321500
C	-2.26425000	-2.09576200	-0.03500100
H	-9.17459800	-0.72744500	-2.20204500
C	-0.92763700	-2.14053800	0.50679400
H	12.77763300	1.47165500	2.33426500
C	-9.60489700	-0.11320000	-1.42343700
C	-4.49899300	-1.69211300	-0.02092800
H	-6.69670500	-0.65792800	-1.27773900
C	-10.83584300	0.59363200	-1.48899400
H	-11.51798500	0.61795700	-2.32734900
N	-6.78725400	-0.82168300	-0.28720500
N	-3.33707800	-1.67305100	0.72533500
C	0.95060200	-2.27259700	1.77577600
H	8.71366100	-0.74186200	2.42776500
H	3.71622300	-1.26413600	1.56535300

C	-5.75645400	-1.24928400	0.52715800
C	-0.46838700	-2.32270300	1.80730800
C	-9.08580900	0.05548400	-0.14398600
H	6.17115300	-1.66448700	2.48599000
C	-7.87666700	-0.43647000	0.46911400
C	-11.05274400	1.18596400	-0.24955500
H	-12.77426500	2.82576100	-1.59989800
H	1.61720100	-2.43562700	2.61112900
N	-12.92760700	2.74923200	-0.60687800
C	-6.20673700	-1.14223200	1.83903400
H	-3.24718100	-1.22143700	1.62231300
N	-9.98291900	0.84193800	0.55213200
C	-12.13142100	2.01030400	0.24489600
C	-7.53287800	-0.63434400	1.80279700
H	-1.08704700	-2.53451900	2.66816600
C	-13.87710400	3.44241100	0.10932200
H	-5.66089400	-1.45174900	2.71931000
C	-12.59722100	2.24061600	1.53479400
H	-9.80459600	1.24072100	1.46065800
C	-13.69477800	3.14324000	1.44523600
H	-8.18689100	-0.48541100	2.65053400
H	-12.21851800	1.77337700	2.43317800
H	-14.29048000	3.51964000	2.26441400
H	15.06478000	4.12179100	-0.24482600
H	-14.59236000	4.08244700	-0.38426300
C	-1.75012500	0.68997400	-1.75745400
O	-0.83098500	0.20975600	-2.29897500
S	-2.97045300	1.36557400	-1.04326900

Low frequencies — 4.4030 9.4409 11.3707

SCF energy — -2393.88768625 A.U.

9Py-CMe			
H	-11.77485800	-1.18095200	-2.57810600
C	-11.18311400	-0.97929400	-1.69602200
C	-9.89492400	-0.37990900	-1.66334700
H	-13.33088300	-2.99797900	-1.45825500
H	-9.32238100	-0.04013500	-2.51503800
N	-13.57711400	-2.63808600	-0.54980800
C	-14.66563600	-3.03086900	0.19608300
H	-4.87337900	1.18590200	-2.28573100
C	-11.58913100	-1.18712000	-0.38239200
C	-4.29548100	1.20441800	-1.37221700
C	-12.79670800	-1.75618900	0.17039600
C	-9.53064900	-0.22823100	-0.32940800
H	-6.96995600	-0.05923500	-1.28830200
C	-2.89192000	1.38553500	-1.26732700
H	-2.19259400	1.49541300	-2.08407600
N	-7.14410600	0.38513600	-0.40047200
N	-10.57519000	-0.71893400	0.42947500
C	-14.59002900	-2.38898900	1.41655700
C	-8.34356600	0.31751000	0.28149400
C	-4.81343800	1.11889700	-0.08299100
H	2.28765800	3.04821900	-1.42621200
C	-13.41521000	-1.58430200	1.40401200
C	-6.16197900	0.94166200	0.39530900
C	2.84305900	2.45443300	-0.71518900
C	-2.56742800	1.41098600	0.08613600
H	-0.03337600	1.50275000	-0.95771200



C	4.23972400	2.18972800	-0.72868900
H	4.95794700	2.57095100	-1.44181900
N	-0.12335800	1.65998500	0.04473200
N	-3.74781700	1.25071800	0.78517100
C	-8.12084700	0.85629200	1.54450000
C	-1.29805000	1.55428700	0.75500900
H	-15.30443300	-2.47706700	2.22250200
H	-10.53346100	-0.86555800	1.42596600
C	-6.75688000	1.24706400	1.61576100
C	2.30654200	1.85033300	0.41621500
H	9.39239800	1.32138100	-1.61192100
C	0.95002200	1.75309300	0.90661500
H	-13.08193000	-0.91764300	2.18713900
C	9.80871100	0.52237900	-1.01437100
C	4.54184700	1.42889100	0.39851700
H	6.87677200	0.89509700	-0.93610900
C	11.08058700	-0.08708500	-1.18847000
H	11.81258200	0.16050400	-1.94454700
N	6.88909100	0.75501500	0.06174100
N	3.35491700	1.24051100	1.07972500
C	-0.96659100	1.59847700	2.10905100
H	-8.87285100	1.00655100	2.30651600
H	-3.81504000	1.14400500	1.78465500
C	5.78875000	0.89321000	0.88540700
C	0.44424800	1.72007000	2.20337300
C	9.22393200	-0.03133100	0.11988900
H	-6.27609500	1.75085500	2.44265900
C	7.95358500	0.21461600	0.75685400
C	11.25640800	-1.00585000	-0.15938800
H	13.15570900	-2.10687300	-1.78985600
H	-1.66123400	1.57192900	2.93725000

N	13.24075100	-2.32034700	-0.80871800
C	6.16721800	0.43461000	2.14334000
H	3.23778800	0.62743100	1.87169100
N	10.12171500	-0.95149300	0.62496100
C	12.34962700	-1.89615700	0.15640800
C	7.52046500	0.01043800	2.06288800
H	1.02472800	1.83081900	3.10880400
C	14.18354100	-3.15541700	-0.25307000
H	5.55362300	0.45435200	3.03313400
C	12.74661700	-2.47689400	1.35598800
H	9.91240700	-1.60375200	1.36457800
C	13.90006100	-3.26944100	1.09378100
H	8.13015300	-0.34943000	2.87975400
H	12.28489300	-2.30969400	2.31915100
H	14.46478500	-3.84623200	1.81210100
H	-15.39198300	-3.72515800	-0.19795800
H	14.96573300	-3.59338800	-0.85409200
C	1.59125100	0.24938000	-2.71278100
O	0.57994500	0.94206300	-2.69810000
C	2.61572700	0.39234300	-3.81328000
H	2.86121700	-0.58234800	-4.24865500
H	2.25080100	1.07051200	-4.58563800
H	3.53733800	0.79412400	-3.37568200
C	1.88565900	-0.76966600	-1.63784800
H	1.95698100	-1.76743100	-2.08685200
H	2.85534400	-0.54777100	-1.17867700
H	1.10783000	-0.76563000	-0.87426500

Low frequencies --- 3.3258 8.2539 10.1345

SCF energy --- -2075.53571486 A.U.
