Electronic Supplementary Information (ESI)

Functionalization and Antioxidant Activity of Polyaniline-fullerene Hybrid Nanomaterials: A Theoretical Investigation

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Figure S1: The IRC plots for all transition states related to reaction of fullerene with aniline at the ONIOM-GD3(B3LYP/6-31G(d):PM6) level of theory in the gas phase.

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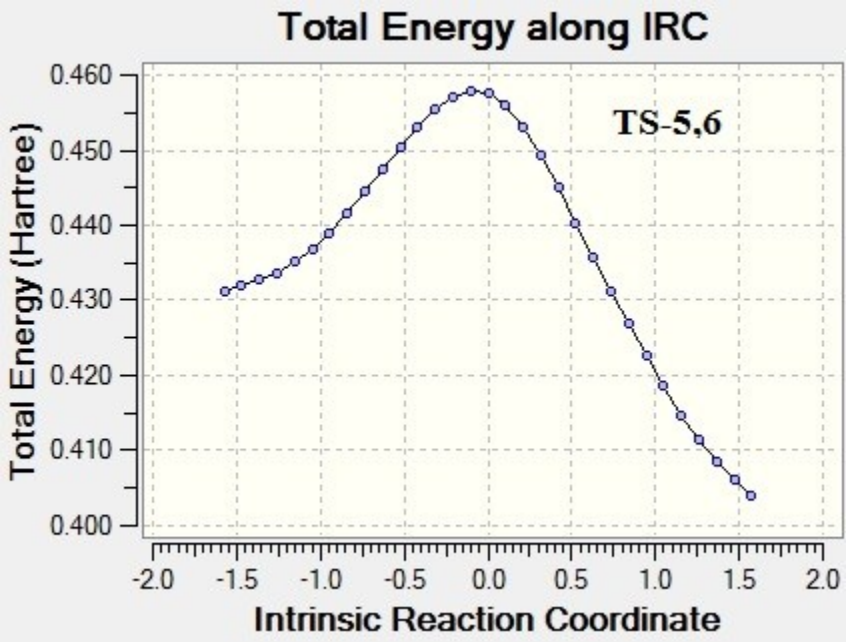
Figure S1*:* The IRC plots for all transition states related to reaction of fullerene with aniline at the ONIOM-GD3(B3LYP/6-31G(d):PM6) level of theory in the gas phase



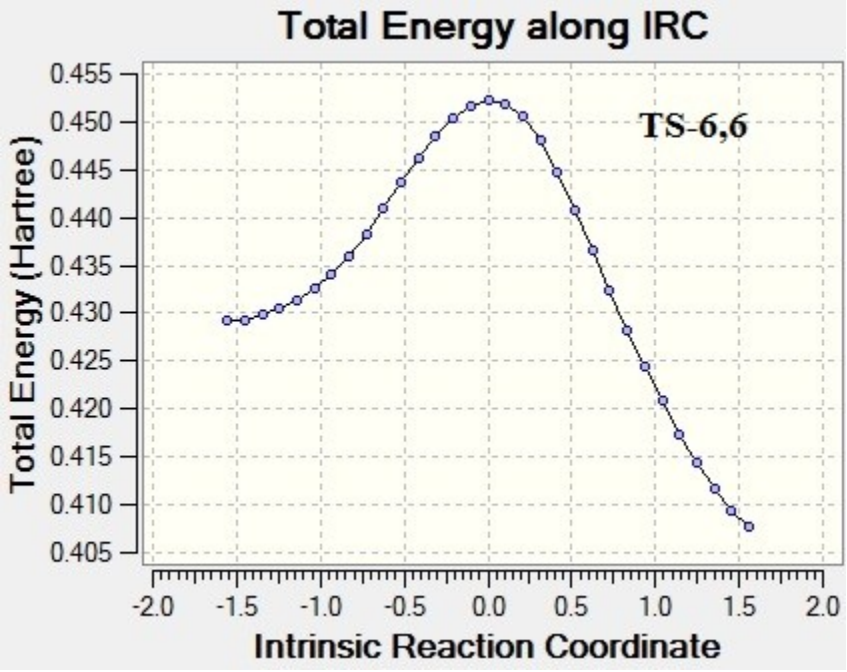


Table S1: Energy barriers (E_a - kcal/mol) and imaginary vibrational frequency (cm^{-1}) of all transition states related to reaction of fullerene with aniline and polyaniline at the ONIOM-GD3(B3LYP/6-31G(d):PM6) method.

Species	E_a	Imaginary frequency
TS(5,6)	48.1	1841.78i
TS(6,6)	36.8	1754.82i
TS-C_{60}-E1	35.8	1763.45i
TS-C_{60}-E2	38.5	1816.70i
TS-C_{60}-L1	35.0	1758.78i
TS-C_{60}-L2	35.4	1815.84i

Table S2: Energies (in Hartree) of all species related to reaction of fullerene with aniline and polyaniline at the ONIOM-GD3(B3LYP/6-31G(d):PM6) level of theory in the gas phase

Species	Energies*	Species	Energies*
C_{60}	-536.785058	**Int-C_{60}-L1**	-1683.207204
Aniline	-287.484207	**Int-C_{60}-L2**	-1683.206417
Int	-824.275667	**TS-C_{60}-E1**	-1681.932314
TS(5,6)	-824.198926	**TS-C_{60}-E2**	-1681.927905
TS(6,6)	-824.216980	**TS-C_{60}-L1**	-1683.151415
P(5,6)	-824.253468	**TS-C_{60}-L2**	-1683.149901
P(6,6)	-824.277023	**P-C_{60}-E1**	-1681.989349
PANI-L	-1146.414446	**P-C_{60}-E2**	-1681.985535
PANI-E	-1145.198447	**P-C_{60}-L1**	-1683.207131
Int-C_{60}-E1	-1681.989375	**P-C_{60}-L2**	-1683.206145
Int-C_{60}-E2	-1681.989234		
** Sum of electronic and zero-point Energies*			

Table S3: Calculated BDE at B3LYP and B3LYP-GD3 level of theory

Compounds	BDE(N–H) (kcal/mol)			Compounds	BDE(N–H) (kcal/mol)		
	B3LYP	B3LYP-GD3	Deviation[a]		B3LYP	B3LYP-GD3	Deviation[a]
PANI-L				**C60-L2**			
N1–H	85.09	85.56	0.47	N1–H	89.78	90.48	0.70
N2–H	78.04	78.86	0.82	N3–H	79.75	80.34	0.59
N3–H	78.10	78.92	0.82	N4–H	81.14	81.73	0.59
N4–H	79.92	80.62	0.70	**C60-E1**			
PANI-E				N1–H	83.86	84.78	0.92
N1–H	86.83	87.28	0.45	N2–H	78.93	79.79	0.86
N2–H	78.66	79.44	0.78	**C60-E2**			
C60-L1				N1–H	90.88	91.48	0.60
N1–H	81.85	82.83	0.98				
N2–H	78.14	79.00	0.86				
N3–H	78.31	79.19	0.88				
N4–H	80.21	80.98	0.77				
[a]Values (B3LYP-GD3/6-311++G(d,p)// B3LYP-GD3/6-31G(d)) – values (B3LYP/6-311++G(d,p)// B3LYP /6-31G(d)							

Table S4: Calculated IE and EA at B3LYP and B3LYP-GD3 level of theory

Compounds	Adiabatic IE (kcal/mol)			Adiabatic EA (kcal/mol)		
	B3LYP	B3LYP-GD3	Deviation[a]	B3LYP	B3LYP-GD3	Deviation[a]
PANI-L	130.36	130.46	0.10	0.58	0.56	-0.02
PANI-E	140.74	140.83	0.09	45.62	45.54	-0.08
C60-L1	130.98	131.22	0.24	65.10	65.06	-0.04
C60-L2	133.97	133.77	-0.20	61.74	61.93	0.19
C60-E1	140.56	140.7	0.14	66.46	66.33	-0.13
C60-E2	143.84	143.8	-0.04	65.18	65.11	-0.07

[a]Values (B3LYP-GD3/6-311++G(d,p)// B3LYP-GD3/6-31G(d)) – values (B3LYP/6-311++G(d,p)// B3LYP /6-31G(d)

Table S5: Cartesian coordinates of all species were calculated at B3LYP/6-311++G(d,p)//B3LYP/6-31G(d) level of theory in the gas phase.

Name of compound	PANI-L		
Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	-4.27091100	-0.49629000	-0.13130600
C	-3.11733200	-0.82695100	-0.85731500
C	-1.84494200	-0.51007000	-0.39030700
C	-1.67918900	0.16444100	0.83124300
C	-2.83661500	0.49658500	1.55830500
C	-4.10549100	0.17108900	1.09354300
H	-3.21907800	-1.32833100	-1.81759000
H	-0.97959900	-0.75734400	-0.99490000
H	-2.73498300	0.99957500	2.51782200
H	-4.97286000	0.41024200	1.69962400
N	-5.52989500	-0.89864100	-0.61325600
H	-5.52817100	-1.72956200	-1.18718100
N	-0.43241100	0.54587800	1.33735900
H	-0.44439600	1.33877500	1.96252300
C	0.84279500	0.08247400	0.97603200
C	1.09223600	-1.25230000	0.61408600
C	1.93850900	0.95707000	1.03910100
C	2.37700700	-1.67102600	0.28904600
H	0.27694400	-1.96775200	0.59416900
C	3.23228900	0.52838600	0.75743100
H	1.77578200	1.99353600	1.32790100
C	3.47578800	-0.79542900	0.35510700
H	2.53924200	-2.70502500	-0.00873800
H	4.05682600	1.22588600	0.85385200
N	4.75034800	-1.28938400	0.05034500
C	5.93333000	-0.56456200	-0.17595900
C	5.95497600	0.63239700	-0.91054800
C	7.15843900	-1.07648100	0.27849500
C	7.15243800	1.29818500	-1.15474000
H	5.02994000	1.03448200	-1.31053400
C	8.35815800	-0.42460100	0.00951500
H	7.17082800	-2.00169300	0.85102700
C	8.37786200	0.78378400	-0.70318900
H	7.13797100	2.22817000	-1.71948200
H	9.29104000	-0.84854000	0.37517100
N	9.57729900	1.48830300	-0.90416000
H	9.56729100	2.09254100	-1.71792700
C	-6.75282400	-0.23103700	-0.53847900
C	-6.86864200	1.12761900	-0.19181100
C	-7.92550600	-0.94375900	-0.85658800

C	-8.12212800	1.73657700	-0.15311100
H	-5.97873600	1.70808200	0.02364700
C	-9.16834600	-0.31962200	-0.82612300
H	-7.85114400	-1.99638500	-1.12297600
C	-9.28156400	1.02574400	-0.46656200
H	-8.18611600	2.78838800	0.11510400
H	-10.05634400	-0.89397500	-1.07831700
H	-10.25324400	1.50958500	-0.43419700
H	4.87643000	-2.27767200	0.21666200
H	10.40296200	0.90059500	-0.91288000

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction= 0.409201
(Hartree/Particle)
Thermal correction to Energy= 0.433518
Thermal correction to Enthalpy= 0.434463
Thermal correction to Gibbs Free Energy= 0.350666

Energy at B3LYP/6-311++G(d,p)

HF= -1147.112052

Name of compound	PANI-L-N1-H radical	
Cartesian Coordinates optimized at B3LYP/6-31G(d)		
C	-4.18529200	-0.44077300	-0.19230900
C	-3.03463500	-0.90820800	-0.84875200
C	-1.77504400	-0.39194400	-0.56411800
C	-1.61739200	0.61757500	0.39951600
C	-2.76668400	1.08445000	1.05649500
C	-4.02693700	0.56955500	0.77106100
H	-3.13350900	-1.67539200	-1.61369500
H	-0.91480700	-0.75032900	-1.11917400
H	-2.66796200	1.85157700	1.82156000
H	-4.88681900	0.92995800	1.32455000
N	-5.42148800	-1.03558600	-0.48132600
H	-5.37531300	-1.98649200	-0.81821700
N	-0.37680500	1.21206000	0.68275800
H	-0.41861500	2.16435500	1.01661300
C	0.89374700	0.63521400	0.68087600
C	1.11270700	-0.75322200	0.73486100
C	2.02102200	1.47811900	0.67141500
C	2.40541800	-1.26540000	0.73611000
H	0.27021800	-1.43352700	0.78400500
C	3.31100000	0.96468700	0.71274300
H	1.87882300	2.55642700	0.64727700
C	3.52687300	-0.42290100	0.72141100
H	2.54914400	-2.34342700	0.75776400
H	4.15583900	1.64401200	0.74928800
N	4.81378400	-0.99199500	0.78370800
C	5.99513000	-0.55222500	0.21331000
C	6.04273500	0.40691700	-0.82836500
C	7.21629600	-1.12049200	0.66448200
C	7.25008900	0.79107800	-1.37079500
H	5.11898000	0.82003600	-1.21822900
C	8.41935400	-0.74238700	0.12163800
H	7.18766000	-1.86016500	1.46282300

C	8.50269800	0.24451900	-0.92227600
H	7.26464900	1.52084500	-2.17794900
H	9.35209300	-1.17399700	0.47121000
N	9.70492800	0.56947900	-1.39477800
H	9.59319500	1.27966200	-2.12944700
C	-6.70699700	-0.49226300	-0.40508900
C	-6.95717600	0.89157800	-0.42606500
C	-7.80369200	-1.37297200	-0.35152400
C	-8.26667500	1.36715300	-0.37495700
H	-6.13157700	1.58953700	-0.50798700
C	-9.10631700	-0.88494700	-0.31643600
H	-7.62324600	-2.44592600	-0.33154500
C	-9.35108000	0.49032800	-0.31882000
H	-8.43678100	2.44077400	-0.39430200
H	-9.93521100	-1.58712300	-0.27728900
H	-10.36763300	0.87035400	-0.28134500
H	4.88305100	-1.84948300	1.31509300

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction= (Hartree/Particle)	0.396781
Thermal correction to Energy=	0.420394
Thermal correction to Enthalpy=	0.421338
Thermal correction to Gibbs Free Energy=	0.338865

Energy at B3LYP/6-311++G(d,p)

HF= -1146.468372

Name of compound	PANI-L-N2-H radical

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	-4.22577200	-0.44109200	-0.19668400
C	-3.09006200	-0.91917100	-0.87174300
C	-1.81608000	-0.44775600	-0.57574200
C	-1.62897600	0.52645200	0.41883400
C	-2.76345200	1.00600400	1.09301700
C	-4.03774800	0.53480700	0.79675800
H	-3.21225900	-1.65888500	-1.65995800
H	-0.96757000	-0.81233200	-1.14397800
H	-2.64108100	1.74565300	1.88128700
H	-4.88590400	0.90123900	1.36412300
N	-5.47784200	-0.99292300	-0.50076100
H	-5.45768900	-1.93497900	-0.86418000
N	-0.37344600	1.07673000	0.72241700
H	-0.39017200	2.02924500	1.05947000
C	0.88763200	0.49448400	0.65205400
C	1.09706100	-0.90232700	0.62147800
C	2.02155200	1.33492200	0.67970800
C	2.37956300	-1.41590200	0.58860900
H	0.24860700	-1.57611500	0.66303100
C	3.30393200	0.81972800	0.62681100
H	1.87860700	2.41228500	0.74798600
C	3.53496100	-0.58544000	0.54976100
H	2.54068200	-2.48973600	0.58706400
H	4.14834100	1.49726600	0.69150200
N	4.74254500	-1.21507000	0.54409900

C	5.90055900	-0.62070100	0.13011600
C	6.02074300	0.44629800	-0.80527000
C	7.11608300	-1.19062200	0.60078500
C	7.25972300	0.92100300	-1.20478300
H	5.12648400	0.85945000	-1.25953400
C	8.35074500	-0.69645200	0.22562500
H	7.04076400	-2.02767000	1.28815100
C	8.44999400	0.37506400	-0.68635600
H	7.31804400	1.72340700	-1.93798000
H	9.25922600	-1.14108800	0.62700800
N	9.69136100	0.90329200	-1.03481800
H	9.72100500	1.40278800	-1.91488300
C	-6.74926400	-0.42299500	-0.39259300
C	-6.96680000	0.96634600	-0.36705100
C	-7.86596000	-1.27911000	-0.35564900
C	-8.26403600	1.47051200	-0.28686500
H	-6.12566500	1.64693300	-0.43585800
C	-9.15622900	-0.76211800	-0.29112800
H	-7.71081000	-2.35606200	-0.37171500
C	-9.36831000	0.61787100	-0.24704400
H	-8.40885700	2.54788800	-0.27025200
H	-10.00110200	-1.44562600	-0.26544100
H	-10.37515400	1.02016200	-0.18656800
H	10.47701800	0.27313900	-0.93170700

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction=	0.396953
(Hartree/Particle)	
Thermal correction to Energy=	0.420511
Thermal correction to Enthalpy=	0.421455
Thermal correction to Gibbs Free Energy=	0.339881

Energy at B3LYP/6-311++G(d,p)

HF= -1146.479721

Name of compound	PANI-L-N3-H radical

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	-4.23648200	-0.39580600	-0.22222200
C	-3.09808800	-0.89837900	-0.88553700
C	-1.82397400	-0.46355000	-0.56339400
C	-1.61244400	0.53138900	0.43336700
C	-2.77654800	1.05430900	1.06017100
C	-4.04663100	0.59020700	0.76936500
H	-3.23086400	-1.62885200	-1.68170300
H	-0.97854000	-0.84212700	-1.12784300
H	-2.63319900	1.82000800	1.81643500
H	-4.89827100	0.97588900	1.31836800
N	-5.48546300	-0.92323500	-0.55093900
H	-5.46452100	-1.83755800	-0.98076700
N	-0.41734600	1.09411600	0.77971300
C	0.77983800	0.46431000	0.63986900
C	1.00668400	-0.94386100	0.59203700
C	1.94197300	1.28804000	0.64408800
C	2.28436500	-1.46289800	0.50042300
H	0.16568400	-1.62352300	0.67626300

C	3.21826400	0.77271100	0.53096600
H	1.78885000	2.35921200	0.73464600
C	3.41977300	-0.62381600	0.44138200
H	2.42476500	-2.54261100	0.47819400
H	4.07250800	1.44019300	0.54722200
N	4.67479500	-1.20862400	0.35643300
C	5.91484000	-0.61321000	0.05182800
C	6.04928400	0.41161600	-0.89801600
C	7.07776300	-1.10092700	0.66673700
C	7.29913800	0.94474100	-1.19619500
H	5.17333200	0.77996100	-1.42130800
C	8.32971600	-0.58588700	0.34875300
H	6.99775600	-1.89392700	1.40697900
C	8.46408600	0.45740300	-0.58159900
H	7.37530300	1.74400700	-1.93025700
H	9.21378900	-0.98310200	0.84256000
N	9.71378200	1.03436300	-0.84397400
H	9.78619600	1.48467500	-1.74859000
C	-6.76281500	-0.37442800	-0.39024100
C	-6.99797200	1.01042900	-0.32529700
C	-7.86419400	-1.24909300	-0.34591900
C	-8.29946600	1.49251400	-0.19534900
H	-6.16901900	1.70432100	-0.40462600
C	-9.15967700	-0.75385900	-0.23254700
H	-7.69294700	-2.32259800	-0.39296800
C	-9.38902600	0.62138500	-0.14642000
H	-8.45998500	2.56660500	-0.14819000
H	-9.99395200	-1.44992300	-0.20128500
H	-10.39951400	1.00676700	-0.04792200
H	4.70931300	-2.19312000	0.58203800
H	10.50250300	0.41932500	-0.68336100
Frequency and Energy at B3LYP/6-31G(d)			
Zero-point correction= 0.397087 (Hartree/Particle)			
Thermal correction to Energy= 0.420603			
Thermal correction to Enthalpy= 0.421547			
Thermal correction to Gibbs Free Energy= 0.340311			
Energy at B3LYP/6-311++G(d,p)			
HF= -1146.479718			

Name of compound	PANI-L-N4-H radical	
Cartesian Coordinates optimized at B3LYP/6-31G(d)		
C	-4.32284300	-0.41263500	-0.33285600
C	-3.12287300	-0.87876200	-0.95459700
C	-1.86893900	-0.53062100	-0.50025400
C	-1.72520100	0.28412200	0.64895700
C	-2.90001300	0.73145600	1.30101800
C	-4.15431600	0.40728700	0.82935200
H	-3.23525000	-1.50380400	-1.83514900
H	-0.98782700	-0.86713100	-1.03480500
H	-2.80339700	1.32691700	2.20740800
H	-5.02974600	0.73714700	1.37780600
N	-5.48915500	-0.84521200	-0.85573000

N	-0.49838700	0.67849100	1.15111200
H	-0.52585000	1.44557100	1.80914500
C	0.78598500	0.17181200	0.86532600
C	1.03069200	-1.19384000	0.64872500
C	1.88143700	1.04715800	0.86079500
C	2.31759700	-1.64856000	0.39208200
H	0.21163700	-1.90382800	0.69204000
C	3.17633900	0.58971700	0.64190200
H	1.71666900	2.10750300	1.03944200
C	3.41938000	-0.77143000	0.38219300
H	2.48014900	-2.70886300	0.21020400
H	4.00254800	1.29046800	0.67759500
N	4.69076600	-1.29298100	0.14826100
C	5.89226300	-0.59572500	-0.08861500
C	5.95722400	0.52110100	-0.93655000
C	7.08732900	-1.06251800	0.47802200
C	7.16873700	1.15995500	-1.18210500
H	5.05610800	0.88024600	-1.42302400
C	8.30310700	-0.44176300	0.20878100
H	7.06317800	-1.92591200	1.13940800
C	8.36599200	0.69101600	-0.61780500
H	7.18956700	2.02897800	-1.83633600
H	9.21357300	-0.82783000	0.66195600
N	9.57616700	1.36946100	-0.82458300
H	9.61419400	1.89929300	-1.68748000
C	-6.70523400	-0.26044100	-0.57083500
C	-6.91669000	1.12938800	-0.38232600
C	-7.84340200	-1.10387600	-0.57704200
C	-8.19899400	1.63261000	-0.18186100
H	-6.07229400	1.80843300	-0.44619800
C	-9.11488900	-0.59515700	-0.34662000
H	-7.68530200	-2.16364000	-0.75289300
C	-9.30392000	0.77748100	-0.14613700
H	-8.33847300	2.70403300	-0.05823400
H	-9.96897200	-1.26787400	-0.33652300
H	-10.30121700	1.17647800	0.01728200
H	4.79117100	-2.28103400	0.33263300
H	10.40121100	0.78987500	-0.72499000

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction= 0.396819
(Hartree/Particle)
Thermal correction to Energy= 0.420440
Thermal correction to Enthalpy= 0.421384
Thermal correction to Gibbs Free Energy= 0.339603

Energy at B3LYP/6-311++G(d,p)

HF= -1146.476656

Name of compound	PANI-L-cation

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	-4.29721200	0.39121100	0.36303000
C	-3.16242600	0.95336500	0.99581000
C	-1.88445800	0.50996700	0.71286200
C	-1.67991600	-0.51805000	-0.23064700

C	-2.80809400	-1.08829700	-0.85586700
C	-4.08721500	-0.64783500	-0.57432400
H	-3.30182500	1.72787400	1.74566500
H	-1.04642300	0.92481800	1.26076400
H	-2.66912900	-1.86941200	-1.59945400
H	-4.92866900	-1.07968600	-1.10186600
N	-5.54132200	0.89367600	0.66690500
H	-5.54588100	1.78268300	1.15048600
N	-0.42140100	-1.03584700	-0.53626600
H	-0.42791200	-1.99044200	-0.87718400
C	0.82878500	-0.45393400	-0.46965100
C	1.03724200	0.94492200	-0.41961600
C	1.96484500	-1.29676900	-0.51790000
C	2.31657200	1.45733200	-0.37003700
H	0.19381700	1.62324700	-0.45827000
C	3.24442400	-0.78543600	-0.46904600
H	1.82657100	-2.37234600	-0.59882900
C	3.45337500	0.61199300	-0.36952300
H	2.45558800	2.53529800	-0.33894800
H	4.09086900	-1.45726300	-0.54031200
N	4.70147300	1.18901500	-0.33002200
C	5.95512600	0.60996200	-0.08142900
C	6.13314300	-0.48041700	0.79076700
C	7.09147200	1.18780100	-0.67892400
C	7.39759000	-0.99470600	1.02481300
H	5.28412600	-0.90002600	1.31897000
C	8.35593600	0.68132300	-0.44020900
H	6.97344700	2.03520100	-1.34991900
C	8.53833400	-0.43242700	0.41031100
H	7.51619000	-1.83139300	1.70800400
H	9.21755300	1.13696300	-0.92029500
N	9.78428300	-0.97009000	0.60942600
H	9.92483100	-1.61230600	1.37618400
C	-6.81824500	0.37159700	0.36014600
C	-7.08679300	-1.00550500	0.38874400
C	-7.85576600	1.27466400	0.08261100
C	-8.37304900	-1.46511300	0.11036200
H	-6.30568800	-1.70718800	0.66135100
C	-9.14008700	0.80454000	-0.17783800
H	-7.64790300	2.34166500	0.06056500
C	-9.40343800	-0.56735700	-0.17511000
H	-8.57297000	-2.53236800	0.13806600
H	-9.93485300	1.51295000	-0.39205100
H	-10.40422500	-0.93227500	-0.38422900
H	4.72218300	2.18154600	-0.53381200
H	10.59820200	-0.43180200	0.34879800

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction= (Hartree/Particle)	0.411766
Thermal correction to Energy=	0.435323
Thermal correction to Enthalpy=	0.436267
Thermal correction to Gibbs Free Energy=	0.355432

Energy at B3LYP/6-311++G(d,p)

HF= -1146.907313

Name of compound	PANI-L-anion		
Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	-4.20381300	-0.04639500	-0.49562800
C	-3.02358400	0.49571400	-1.06245200
C	-1.77035400	0.23478400	-0.53625800
C	-1.62234700	-0.59482200	0.61097800
C	-2.80770700	-1.13730000	1.17863000
C	-4.05780000	-0.87712300	0.64723300
H	-3.11060800	1.15150100	-1.92849500
H	-0.89409900	0.69239200	-0.98364900
H	-2.72258400	-1.79075200	2.04707300
H	-4.93740800	-1.33120500	1.09504500
N	-5.44694800	0.17991400	-1.12514200
H	-5.43752300	0.17542700	-2.13825900
N	-0.39364600	-0.84043900	1.23205800
H	-0.44741900	-1.02865100	2.22587200
C	0.88508900	-0.91182400	0.69504600
C	1.14417000	-1.08484600	-0.70008500
C	2.00076900	-0.84122100	1.56320000
C	2.45298800	-1.14893400	-1.16058200
H	0.31729600	-1.17722500	-1.39430900
C	3.30031300	-0.94765800	1.09535100
H	1.82377300	-0.71753600	2.63258500
C	3.55701000	-1.08173800	-0.29725200
H	2.63944600	-1.26965300	-2.22658900
H	4.13335000	-0.91937900	1.79327600
N	4.88277000	-1.21988800	-0.81637700
C	5.93211200	-0.35928400	-0.48888200
C	5.71133500	0.95494500	-0.02704500
C	7.26478300	-0.77244800	-0.66229800
C	6.78935800	1.80303600	0.24293400
H	4.69458200	1.30185900	0.11831800
C	8.33550700	0.08481300	-0.40457400
H	7.46396800	-1.78402800	-1.01520900
C	8.11271400	1.38954200	0.06156300
H	6.58999500	2.81138300	0.60503900
H	9.35447800	-0.26056400	-0.57346800
N	9.20596300	2.27780400	0.28366000
H	8.95400500	3.01707500	0.93369000
C	-6.68253300	0.41592000	-0.55400200
C	-6.85008100	0.73284700	0.82132300
C	-7.84577900	0.35754700	-1.36127900
C	-8.12023800	0.97007300	1.33482000
H	-5.97692400	0.80248600	1.46009000
C	-9.10388100	0.60937800	-0.83197200
H	-7.73897700	0.11367700	-2.41838400
C	-9.26596600	0.91261500	0.53122900
H	-8.21646700	1.21465200	2.39200700
H	-9.97228700	0.56526700	-1.48755500
H	-10.25246600	1.09261000	0.94985100
H	5.19358300	-2.17551800	-0.96832200
H	10.01292500	1.78872200	0.66202300

Frequency and Energy at B3LYP/6-31G(d)	
Zero-point correction= (Hartree/Particle)	0.400637
Thermal correction to Energy=	0.425671
Thermal correction to Enthalpy=	0.426615
Thermal correction to Gibbs Free Energy=	0.341426
Energy at B3LYP/6-311++G(d,p)	
HF= -1147.103926	

Name of compound	PANI-E		
Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	-4.28913700	0.35166500	0.42104600
C	-3.06745000	0.85662900	1.04621100
C	-1.83309100	0.54624400	0.58983200
C	-1.65361300	-0.30706800	-0.58394800
C	-2.87223300	-0.83694500	-1.18812600
C	-4.10850400	-0.51967900	-0.74080300
H	-3.20760500	1.46602900	1.93426200
H	-0.95348600	0.89066000	1.12223000
H	-2.73068600	-1.46855400	-2.06041000
H	-4.99026200	-0.88796300	-1.25343900
N	-5.41787900	0.73322900	0.94937700
N	-0.52654200	-0.67346400	-1.13701400
C	0.71502100	-0.13666100	-0.83257300
C	0.97715500	1.22336700	-0.54394400
C	1.82925600	-0.99730800	-0.93922400
C	2.26933100	1.67014300	-0.31805800
H	0.16326600	1.94115800	-0.54944300
C	3.11984500	-0.56469300	-0.68257200
H	1.64602400	-2.03029700	-1.21959200
C	3.36789800	0.78557200	-0.35496100
H	2.44360900	2.72483000	-0.11318800
H	3.94776900	-1.25834000	-0.77400300
N	4.63840900	1.29045000	-0.12406000
C	5.84587700	0.58973800	0.08187500
C	5.91849100	-0.57051400	0.86764800
C	7.03556800	1.09734600	-0.46003600
C	7.13472700	-1.21294300	1.07630300
H	5.01983200	-0.96502600	1.33039700
C	8.25569300	0.47138100	-0.22814900
H	7.00174400	1.99237000	-1.07708900
C	8.32747300	-0.70472800	0.53584600
H	7.16485500	-2.11043700	1.69021600
H	9.16415000	0.89293900	-0.65257700
N	9.55908200	-1.31375100	0.80793100
H	9.50130000	-2.30183100	1.02315600
C	-6.65874600	0.21782400	0.56881800
C	-6.93457200	-1.16273200	0.48739500
C	-7.71733000	1.12693900	0.37371600
C	-8.22145400	-1.60973000	0.19138400
H	-6.14265100	-1.87599200	0.69626200
C	-8.99162400	0.67226800	0.05045100
H	-7.50895900	2.18828000	0.46949700

C	-9.25306800	-0.69853600	-0.04170700
H	-8.41788700	-2.67802600	0.14540400
H	-9.79050300	1.39041200	-0.11611900
H	-10.25331700	-1.05137500	-0.27685400
H	4.72000300	2.29660300	-0.16786000
H	10.27823100	-1.13616500	0.11696500

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction= 0.385943
(Hartree/Particle)
Thermal correction to Energy= 0.409013
Thermal correction to Enthalpy= 0.409957
Thermal correction to Gibbs Free Energy= 0.330378

Energy at B3LYP/6-311++G(d,p)

HF= -1145.863814

Name of compound	PANI-E-N1-H radical

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	-4.16846900	0.29514200	0.45801900
C	-2.90822300	0.68729400	1.08917900
C	-1.70461800	0.43644000	0.52847400
C	-1.60164600	-0.22708000	-0.77186100
C	-2.85959000	-0.63357300	-1.39486100
C	-4.06426800	-0.37882100	-0.83795900
H	-2.99401500	1.15712000	2.06456300
H	-0.79188300	0.68991100	1.05634500
H	-2.77294600	-1.11572800	-2.36415900
H	-4.97797200	-0.64597700	-1.35713600
N	-5.26025200	0.59627600	1.10088100
N	-0.50965200	-0.51774400	-1.42517100
C	0.75504900	-0.05742200	-1.08054000
C	1.05014200	1.26373000	-0.67676200
C	1.84066000	-0.93719300	-1.27469700
C	2.35722300	1.65599500	-0.42434700
H	0.25054200	1.99360700	-0.60070200
C	3.14549100	-0.55627800	-1.00228300
H	1.62917400	-1.93492300	-1.64666900
C	3.42502500	0.75012700	-0.55573100
H	2.56056500	2.67951000	-0.11619800
H	3.95626500	-1.25320500	-1.18079000
N	4.72393600	1.21130100	-0.31496100
C	5.86423900	0.51525900	0.05868200
C	5.82934800	-0.76257300	0.67270400
C	7.12224700	1.14022900	-0.13499900
C	6.99654000	-1.38930200	1.04390400
H	4.87484000	-1.23299500	0.87928000
C	8.28987400	0.51794100	0.23991100
H	7.15549700	2.12293800	-0.60211100
C	8.28802000	-0.79000700	0.84086500
H	6.97526800	-2.36207600	1.52520900
H	9.24386400	1.01408900	0.07503500
N	9.36845100	-1.46675300	1.22457200
C	-6.52920700	0.15877800	0.71520600
C	-6.82951100	-1.18501700	0.41104900

C	-7.58233300	1.09400500	0.74946100
C	-8.13853700	-1.56632600	0.12089600
H	-6.03887300	-1.92863000	0.44676200
C	-8.87991700	0.70999900	0.42802900
H	-7.35180400	2.12040000	1.01814800
C	-9.16685100	-0.62218800	0.11320400
H	-8.35488000	-2.60896200	-0.09748000
H	-9.67614100	1.44974500	0.43876800
H	-10.18459000	-0.92316000	-0.11858800
H	4.85004800	2.20827000	-0.43094600
H	10.20552900	-0.90644800	1.02017200

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction= 0.373263
(Hartree/Particle)
Thermal correction to Energy= 0.395721
Thermal correction to Enthalpy= 0.396666
Thermal correction to Gibbs Free Energy= 0.317776

Energy at B3LYP/6-311++G(d,p)

HF= -1145.217201

Name of compound	PANI-E-N2-H radical	

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	4.23503500	0.37883500	-0.40923600
C	3.01798700	0.89246900	-1.01917000
C	1.78026600	0.53116600	-0.59290800
C	1.61041600	-0.38134900	0.52352800
C	2.82013800	-0.91349700	1.11812400
C	4.06002200	-0.54627800	0.70241600
H	3.15223800	1.55511700	-1.86894200
H	0.90028700	0.88763800	-1.11703300
H	2.68471700	-1.59205200	1.95525900
H	4.94062400	-0.91835400	1.21409100
N	5.36938900	0.81385100	-0.90539000
N	0.46537300	-0.82021900	1.02392800
C	-0.75715400	-0.26158900	0.82254300
C	-1.02058700	1.12993200	0.61502000
C	-1.88653000	-1.12432200	0.96284700
C	-2.30730000	1.59110100	0.49276100
H	-0.19436600	1.83312300	0.62265500
C	-3.17020400	-0.67806800	0.77082100
H	-1.68833500	-2.16214500	1.21376600
C	-3.43846600	0.70775000	0.49517500
H	-2.51313400	2.65012700	0.37059600
H	-4.00118500	-1.36273100	0.89962600
N	-4.64234400	1.28135400	0.34097300
C	-5.78614800	0.60350200	0.01703600
C	-5.86912900	-0.59567600	-0.74395200
C	-7.01494100	1.21352400	0.38709900
C	-7.09137400	-1.15896700	-1.06743000
H	-4.96119500	-1.04997900	-1.12577100
C	-8.23407600	0.63414900	0.09486600
H	-6.96410200	2.14804500	0.93706900
C	-8.29907100	-0.57112500	-0.63721200

H	-7.12626900	-2.05936700	-1.67715900
H	-9.15616200	1.11609500	0.41230300
N	-9.52103100	-1.12058900	-0.99206000
H	-9.52346200	-2.10306500	-1.23220300
C	6.61208100	0.28905500	-0.55984200
C	6.89393000	-1.09335000	-0.50430000
C	7.67427000	1.19788000	-0.37164500
C	8.18673200	-1.54044500	-0.23844400
H	6.10274100	-1.80652700	-0.71510200
C	8.95418900	0.74228500	-0.07589400
H	7.46069200	2.25958900	-0.44907300
C	9.21971100	-0.62951600	-0.00823400
H	8.38785700	-2.60853800	-0.21470200
H	9.75450800	1.45948800	0.08723400
H	10.22466700	-0.98332000	0.20420100
H	-10.31861300	-0.84870200	-0.43277200

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction= (Hartree/Particle)	0.372349
Thermal correction to Energy=	0.394990
Thermal correction to Enthalpy=	0.395934
Thermal correction to Gibbs Free Energy=	0.317035

Energy at B3LYP/6-311++G(d,p)

HF= -1145.229488

Name of compound	PANI-E-cation

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	-4.27284900	0.36910000	0.35124300
C	-3.05896400	0.87763800	0.97096600
C	-1.82352700	0.49117500	0.56445500
C	-1.66462400	-0.42023700	-0.55574200
C	-2.87240200	-0.91626100	-1.19062100
C	-4.10759500	-0.53574700	-0.77912600
H	-3.19573500	1.54858000	1.81341600
H	-0.93972200	0.83267300	1.09264000
H	-2.73674200	-1.57203300	-2.04488800
H	-4.98780200	-0.86595100	-1.31871000
N	-5.40048000	0.80956700	0.85601500
N	-0.51908900	-0.87213100	-1.02435700
C	0.71008400	-0.33416000	-0.82080100
C	0.98666900	1.06487100	-0.75654700
C	1.82288000	-1.22519600	-0.81503200
C	2.27834500	1.52230500	-0.63394400
H	0.17112600	1.77431900	-0.84552000
C	3.11250200	-0.77367800	-0.65775800
H	1.62163400	-2.28329900	-0.94490800
C	3.36852800	0.61771800	-0.54408100
H	2.46979300	2.59223600	-0.59162100
H	3.93540400	-1.47732100	-0.68583600
N	4.63271700	1.14615400	-0.41668100
C	5.83591300	0.55644400	-0.03876600
C	5.91314600	-0.58470300	0.78977000
C	7.03703000	1.17288100	-0.45635500

C	7.13958100	-1.10730000	1.14818800
H	5.01047700	-1.03102300	1.18964900
C	8.26306500	0.65333000	-0.10070600
H	6.99507800	2.05825000	-1.08601600
C	8.34612600	-0.51112600	0.70376200
H	7.18183500	-1.97476100	1.80070900
H	9.17411700	1.13533200	-0.44328200
N	9.55105000	-1.03688300	1.04618700
H	9.61971400	-1.83601700	1.65841200
C	-6.65150600	0.29983000	0.56748900
C	-6.93481200	-1.07410500	0.36701500
C	-7.72473000	1.22192100	0.58348400
C	-8.24212700	-1.49093400	0.14559100
H	-6.13849000	-1.80594600	0.45629000
C	-9.01954600	0.79896600	0.31817300
H	-7.50023700	2.26506800	0.78085100
C	-9.28428600	-0.55852200	0.09924700
H	-8.45421200	-2.54856100	0.01864700
H	-9.83097700	1.52042500	0.30329900
H	-10.30214900	-0.89165700	-0.08017200
H	4.70190100	2.13317000	-0.64286200
H	10.41419600	-0.58568900	0.78233600

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction= 0.386525
(Hartree/Particle)
Thermal correction to Energy= 0.409694
Thermal correction to Enthalpy= 0.410638
Thermal correction to Gibbs Free Energy= 0.330591

Energy at B3LYP/6-311++G(d,p)

HF= -1145.641406

Name of compound	PANI-E-anion	
Cartesian Coordinates optimized at B3LYP/6-31G(d)		
C	-4.14471000	-0.36720600	0.37317100
C	-2.86828600	-0.92020100	0.73128900
C	-1.67431400	-0.34730600	0.36666000
C	-1.62006100	0.87215400	-0.39582100
C	-2.89602100	1.42309500	-0.75702000
C	-4.09011900	0.85152000	-0.39172000
H	-2.88561300	-1.84874400	1.29789700
H	-0.74446100	-0.84348000	0.62928400
H	-2.87829800	2.35018500	-1.32606600
H	-5.02062900	1.34426400	-0.65813000
N	-5.24308100	-0.99355400	0.83168100
N	-0.52124400	1.50285800	-0.85232700
C	0.73817100	1.29840800	-0.35604100
C	1.07332100	1.01296400	0.99755200
C	1.83885100	1.50894900	-1.23304200
C	2.39609500	0.90528800	1.41454800
H	0.27612900	0.90104200	1.72544400
C	3.15627900	1.41423500	-0.81037600
H	1.60980100	1.76691200	-2.26358600
C	3.46220700	1.09105100	0.52361300

H	2.61140900	0.67683700	2.45862500
H	3.96662100	1.60932800	-1.50889000
N	4.80535700	1.04551400	0.98837200
C	5.81958000	0.21487300	0.50233900
C	5.64307800	-0.67772200	-0.56963000
C	7.09634200	0.27251500	1.09358700
C	6.70078100	-1.46039300	-1.02885500
H	4.66996600	-0.76073700	-1.04048900
C	8.14385700	-0.52300500	0.64030400
H	7.26662400	0.95880000	1.92152900
C	7.96924400	-1.40083400	-0.43849500
H	6.52901200	-2.14356000	-1.85941800
H	9.11426000	-0.45987800	1.13045100
N	9.02475100	-2.24585400	-0.87099600
H	8.91951600	-2.52141200	-1.84237500
C	-6.50662200	-0.77178700	0.34548300
C	-6.83931700	-0.52033600	-1.01533700
C	-7.59854000	-0.91830600	1.24410500
C	-8.16412000	-0.40530400	-1.42806900
H	-6.03902800	-0.45305600	-1.74600600
C	-8.91611500	-0.78600700	0.82464000
H	-7.36225200	-1.13418900	2.28291400
C	-9.21910000	-0.52435600	-0.51782900
H	-8.37670100	-0.22382600	-2.48113500
H	-9.72120000	-0.89361600	1.55064900
H	-10.25117500	-0.42739300	-0.84684100
H	4.91638800	1.30070100	1.96058700
H	9.93626500	-1.81466500	-0.75187900

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction=	0.382852
(Hartree/Particle)	
Thermal correction to Energy=	0.406107
Thermal correction to Enthalpy=	0.407051
Thermal correction to Gibbs Free Energy=	0.326233

Energy at B3LYP/6-311++G(d,p)

HF= -1145.932413

Name of compound	C60-E1

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	-2.55663100	-0.13909400	2.85063700
C	-3.57596000	0.86523400	3.09353200
C	-4.88646700	0.47337500	3.39473500
C	-5.22787900	-0.93940700	3.44373800
C	-4.24843200	-1.90383000	3.21021100
C	-2.88311100	-1.49910300	2.91662600
C	-1.66099500	0.36297500	1.84420800
C	-1.93412300	1.84757600	1.58703800
C	-3.31382200	1.99125200	2.23859300
C	-4.36970200	2.66126700	1.66351000
C	-5.99150500	1.18542500	2.80111600
C	-6.55367300	-1.09543700	2.87079000
C	-6.84567100	-2.21034400	2.08267300
C	-5.82413200	-3.21620900	1.83920200

C	-4.55155600	-3.06649500	2.39351100
C	-3.37252900	-3.37498800	1.60049900
C	-2.34519800	-2.40404700	1.93044900
C	-1.50721800	-1.90365800	0.92783500
C	-1.16175600	-0.50029100	0.89356300
C	-1.83451700	2.32450000	0.06299800
C	-1.51875400	1.16433700	-0.91778700
C	-1.09923800	-0.08779500	-0.52804600
C	-1.40584300	-1.25195100	-1.33023100
C	-1.65783200	-2.36952300	-0.43903100
C	-2.63471900	-3.31318300	-0.75548500
C	-3.51546000	-3.82069900	0.28471300
C	-4.83723600	-3.97845800	-0.28945100
C	-5.97005700	-3.68178500	0.47149900
C	-7.02508000	0.22081700	2.47142000
C	-7.49647700	-1.26643900	-1.87244000
C	-8.01065600	-0.38870300	-0.91547400
C	-7.66429300	1.01806400	-0.96173000
C	-6.82144400	1.49894500	-1.96616100
C	-6.28707900	0.58623800	-2.96385400
C	-5.59593700	-1.77499900	-3.15957300
C	-5.84513200	-2.89251000	-2.26618600
C	-7.02056000	-2.57947100	-1.47134000
C	-7.08121400	-2.96514400	-0.13119500
C	-7.62155400	-2.05568900	0.86504700
C	-8.07450700	-0.79138600	0.48220000
C	-7.50880900	1.48571500	0.40694100
C	-6.50557900	2.40306300	0.71795200
C	-5.62533400	2.90116600	-0.32291500
C	-5.78513300	2.46130600	-1.64099300
C	-4.61795300	2.14913700	-2.42943600
C	-4.92204600	0.98985300	-3.25318900
C	-3.94239600	0.02639000	-3.48481300
C	-4.28488800	-1.38437900	-3.44012200
C	-4.77355700	-3.57554100	-1.68716200
C	-3.41249500	-3.16830100	-1.97564400
C	-3.16965600	-2.09565000	-2.83668300
C	-2.14260300	-1.12319800	-2.51179800
C	-2.61576000	0.18160700	-2.90719300
C	-2.32295700	1.28973000	-2.10445600
C	-3.34839500	2.28914300	-1.85856300
C	-3.18795200	2.78443500	-0.51902600
C	-4.30221400	3.06075300	0.23954000
C	-7.76958000	0.36703400	1.29894400
C	-5.72980000	2.25458900	1.93687900
C	-6.61752400	-0.76957900	-2.91633300
C	0.48255200	3.40835400	0.03113200
C	1.20008600	2.35371700	0.61752000
C	2.59163600	2.39185500	0.70367400
C	3.32164200	3.46702100	0.18139700
C	2.60541800	4.52056800	-0.41032700
C	1.21981900	4.49664500	-0.47371700
H	0.68843800	1.49433900	1.03237300
H	3.10904800	1.57823900	1.20046400

H	3.14578400	5.36509700	-0.83177500
H	0.69377400	5.33220500	-0.93103800
N	-0.91912400	3.47454600	-0.02678000
H	-1.20810600	2.47038400	2.12462600
H	-1.24609300	4.16624700	-0.68940500
N	4.72301600	3.56265900	0.27644600
H	5.08693700	4.49788500	0.39368300
C	5.67604800	2.55310400	0.24951700
C	6.97543500	2.83625500	0.71913300
C	5.41662300	1.25667900	-0.24242500
C	7.98176800	1.88463600	0.66921200
H	7.18410300	3.81573600	1.14483000
C	6.41440700	0.29527300	-0.24443400
H	4.43333000	1.01067300	-0.62665300
C	7.73220700	0.58432500	0.17204700
H	8.95769600	2.12462100	1.07902400
H	6.20485300	-0.70617900	-0.60774300
N	8.64463000	-0.46026200	0.16446900
C	9.92110200	-0.32889400	-0.08414100
C	10.74794900	-1.51221700	0.13499900
C	10.60618000	0.84527400	-0.62484900
C	12.09206700	-1.50018900	-0.01164300
H	10.21946000	-2.40727200	0.45037500
C	11.94358000	0.84291800	-0.82275000
H	10.01285500	1.70423100	-0.91804500
C	12.78922800	-0.29585600	-0.46705200
H	12.67405300	-2.39697800	0.16999500
H	12.45608000	1.69741400	-1.25506200
N	14.07102000	-0.15315200	-0.65290400
C	15.01554700	-1.10146700	-0.25412100
C	16.05207700	-1.41619500	-1.15495200
C	15.05217000	-1.66593400	1.03767200
C	17.05577900	-2.30992000	-0.79591200
H	16.03856200	-0.95408200	-2.13742500
C	16.07816500	-2.53794900	1.39832900
H	14.29397700	-1.38432100	1.76247800
C	17.07669000	-2.87567300	0.48290100
H	17.83582600	-2.55577000	-1.51192600
H	16.09726600	-2.95341500	2.40277000
H	17.87177700	-3.55939600	0.76685300

Frequency and Energy at B3LYP/6-31G(d)	
Zero-point correction=	0.763451 (Hartree/Particle)
Thermal correction to Energy=	0.808344
Thermal correction to Enthalpy=	0.809288
Thermal correction to Gibbs Free Energy=	0.686131

Energy at B3LYP/6-311++G(d,p)
HF= -3432.463447

Name of compound	C60-E1-N1-H radical

Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	2.32945700	-0.46692000	-2.65584800
C	3.27050300	0.54707500	-3.09513800
C	4.56293400	0.17697300	-3.48894400

C	4.96552000	-1.21948100	-3.43686200
C	4.06102100	-2.19348200	-3.01600900
C	2.71323300	-1.81337200	-2.62491400
C	1.50974200	0.09820300	-1.61806800
C	1.73202400	1.61192600	-1.53662600
C	3.03603600	1.74291100	-2.33178200
C	4.11030300	2.50258800	-1.92605000
C	5.68410200	0.98599000	-3.07946500
C	6.34667700	-1.26683900	-2.98851000
C	6.76680500	-2.28601400	-2.13157100
C	5.82312200	-3.30122300	-1.69183600
C	4.49719000	-3.25658800	-2.12696300
C	3.41659900	-3.53016200	-1.19328000
C	2.31716400	-2.63636200	-1.50829400
C	1.55657400	-2.07155800	-0.47860900
C	1.14868600	-0.68596000	-0.54364000
C	1.75381700	2.23570100	-0.05370200
C	1.59782200	1.16298100	1.05674900
C	1.20319200	-0.13734300	0.83213700
C	1.64229900	-1.20306300	1.70588000
C	1.86086900	-2.39302100	0.90410200
C	2.90792400	-3.26259400	1.20876700
C	3.70739800	-3.83676100	0.13799300
C	5.08447500	-3.88579500	0.58851800
C	6.12267100	-3.62237400	-0.30758900
C	6.79036400	0.09978100	-2.76576900
C	7.75126300	-0.92914900	1.63023500
C	8.12672800	-0.13132800	0.54706800
C	7.72079000	1.25934000	0.49389800
C	6.95499300	1.80487900	1.52703300
C	6.56407300	0.97500900	2.65556700
C	6.00998400	-1.37982200	3.14442900
C	6.22508000	-2.57023400	2.34104600
C	7.30190500	-2.29259700	1.40537500
C	7.25168500	-2.80767400	0.10892200
C	7.64849900	-1.98147900	-1.01860900
C	8.07439800	-0.66862100	-0.80516400
C	7.41039200	1.58158000	-0.88972800
C	6.33738100	2.42335600	-1.18290600
C	5.53896700	2.98959000	-0.11126500
C	5.84917600	2.69249000	1.22017400
C	4.77857100	2.41290800	2.14608900
C	5.21547500	1.35299800	3.04069400
C	4.31045600	0.38040200	3.46194000
C	4.71486500	-1.01360000	3.51697300
C	5.13676700	-3.34872300	1.94090900
C	3.79198600	-2.96767500	2.32529700
C	3.58222400	-1.82414400	3.09984300
C	2.48303000	-0.92894900	2.78923500
C	2.92889900	0.42595300	3.00841800
C	2.50852300	1.43712200	2.13643200
C	3.45460400	2.44667700	1.69388500
C	3.14156600	2.79166100	0.33686400
C	4.16154700	3.04449600	-0.54922700

C	7.63628000	0.39037100	-1.69320900
C	5.45536700	2.12403600	-2.29729600
C	6.95384500	-0.36490900	2.70483200
C	-0.50130500	3.22654800	-0.02949400
C	-1.27579900	2.04506200	-0.29326500
C	-2.65377000	2.07881300	-0.36198800
C	-3.36475000	3.28600200	-0.16390600
C	-2.62204400	4.47249200	0.07208900
C	-1.25214000	4.44385500	0.13364700
H	-0.78133300	1.09831700	-0.46647700
H	-3.19507700	1.17140300	-0.60431600
H	-3.15440100	5.41014400	0.21944300
H	-0.68189000	5.34753100	0.32275900
N	0.82593800	3.36249800	0.06662300
H	0.92633000	2.14291100	-2.05958400
N	-4.74288300	3.38057500	-0.23969400
H	-5.09942300	4.31667700	-0.38206600
C	-5.72265800	2.38009200	-0.17010100
C	-6.94451700	2.59248300	-0.83236100
C	-5.55377800	1.19301400	0.56708400
C	-7.97261400	1.66405400	-0.74928600
H	-7.07704700	3.48958600	-1.43304200
C	-6.56551400	0.24525800	0.60710400
H	-4.63630100	1.02216600	1.11869000
C	-7.81009100	0.46607800	-0.01886800
H	-8.89212700	1.83506500	-1.30010200
H	-6.42678500	-0.67818600	1.16043100
N	-8.74892100	-0.55742500	0.03134900
C	-10.03045700	-0.36832800	0.18363900
C	-10.88377800	-1.54736500	0.04536500
C	-10.70220100	0.88075500	0.54790000
C	-12.23132600	-1.48086500	0.11625500
H	-10.36926200	-2.48628600	-0.13678300
C	-12.04666900	0.93747900	0.66811500
H	-10.09488400	1.75221500	0.76631600
C	-12.90935000	-0.21245600	0.39574800
H	-12.83360000	-2.37573600	0.00580800
H	-12.55393700	1.85059400	0.96543700
N	-14.19223600	-0.01215500	0.48997800
C	-15.15016500	-0.96772200	0.14383200
C	-16.25447200	-1.12704200	1.00396000
C	-15.12810400	-1.68806200	-1.06825900
C	-17.26981900	-2.02481400	0.69166400
H	-16.28338100	-0.54404600	1.91939700
C	-16.16624500	-2.56168900	-1.38726600
H	-14.31642500	-1.52414300	-1.77087500
C	-17.23318800	-2.74630000	-0.50593600
H	-18.10354500	-2.15122000	1.37729300
H	-16.14132000	-3.09841300	-2.33213600
H	-18.03743300	-3.43216300	-0.75660600

Frequency and Energy at B3LYP/6-31G(d)	
Zero-point correction=	0.750461 (Hartree/Particle)
Thermal correction to Energy=	0.795032
Thermal correction to Enthalpy=	0.795976

Thermal correction to Gibbs Free Energy= 0.673119
Energy at B3LYP/6-311++G(d,p)
HF= -3431.821546

Name of compound	C60-E1-N2-H radical

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	2.45546200	-0.37127400	-2.78663800
C	3.43373500	0.64239200	-3.13580500
C	4.74340400	0.26768500	-3.46111200
C	5.12563500	-1.13508200	-3.42996900
C	4.18547000	-2.10842900	-3.09438400
C	2.82059900	-1.72288500	-2.77454200
C	1.58358700	0.17204900	-1.78091400
C	1.82027600	1.67765600	-1.63453300
C	3.16970700	1.81602800	-2.34801600
C	4.22577800	2.55189400	-1.86014800
C	5.84783400	1.04866400	-2.96031100
C	6.47619600	-1.21513900	-2.90093100
C	6.83119600	-2.26570900	-2.05263200
C	5.85059600	-3.28088300	-1.70276800
C	4.55417800	-3.20466100	-2.21516800
C	3.41568600	-3.49158500	-1.35740200
C	2.34767100	-2.57395000	-1.71011000
C	1.53304300	-2.03062000	-0.71062100
C	1.14670900	-0.63818600	-0.75616600
C	1.76574600	2.25300200	-0.14099700
C	1.52006900	1.15455000	0.92730500
C	1.12678100	-0.13228400	0.63627000
C	1.49778000	-1.23072700	1.50134400
C	1.74935200	-2.39850300	0.67709700
C	2.76562100	-3.29108100	1.01657600
C	3.62157900	-3.84307900	-0.02158100
C	4.96816100	-3.92484900	0.50909900
C	6.06197800	-3.64888300	-0.31404100
C	6.92199100	0.13760800	-2.60854000
C	7.60120600	-1.03956500	1.80231000
C	8.05236800	-0.21441000	0.76977400
C	7.66527300	1.18208200	0.73627000
C	6.84675800	1.70598100	1.73928900
C	6.37821600	0.84810300	2.81559000
C	5.76697100	-1.51279800	3.19466200
C	6.01615900	-2.68062900	2.36808800
C	7.15072800	-2.38932000	1.50831600
C	7.17278400	-2.86273000	0.19536800
C	7.64735700	-2.00785100	-0.87961800
C	8.07569400	-0.70852700	-0.59954000
C	7.44421100	1.55170100	-0.65323100
C	6.40274100	2.41777200	-0.98452600
C	5.54775400	2.96019600	0.05507700
C	5.76999800	2.61476100	1.39204500
C	4.64347800	2.32441800	2.24550700
C	5.01349700	1.23219700	3.13147200
C	4.07295900	0.25980300	3.46507900

C	4.45618700	-1.14074700	3.50032500
C	4.94483100	-3.43069400	1.87845400
C	3.58387600	-3.04283900	2.19287200
C	3.34128900	-1.92178700	2.98994600
C	2.27400400	-1.00213500	2.64169400
C	2.72151300	0.33892700	2.93125900
C	2.36492600	1.38225900	2.06971300
C	3.34965100	2.39043800	1.71788700
C	3.12462500	2.78996700	0.35596400
C	4.20011300	3.04355300	-0.46395100
C	7.70513700	0.38312500	-1.47859500
C	5.58656900	2.16606400	-2.15938900
C	6.74765600	-0.49806200	2.84505100
C	-0.56676200	3.31792400	-0.12971600
C	-1.29250800	2.19111800	-0.56664300
C	-2.67963300	2.21438800	-0.61430200
C	-3.42111200	3.36713600	-0.24708000
C	-2.67012400	4.51288600	0.13179300
C	-1.29466100	4.48269600	0.21487100
H	-0.77941800	1.29075100	-0.88108800
H	-3.20163800	1.34402300	-0.99719400
H	-3.21960600	5.41500600	0.38195600
H	-0.75286300	5.37155200	0.53218200
N	0.81893600	3.37568500	-0.07719100
H	1.05321100	2.23872600	-2.18314200
H	1.18478300	4.18780100	0.40040100
N	-4.78004700	3.51856600	-0.32282400
C	-5.66327100	2.51819300	-0.18650100
C	-6.99825100	2.78002100	-0.64548000
C	-5.43020100	1.23425200	0.41930400
C	-8.00097000	1.84948300	-0.54477200
H	-7.17339600	3.74199400	-1.11761200
C	-6.43435000	0.30392500	0.51363500
H	-4.45701400	1.01831500	0.84603600
C	-7.76209000	0.57481800	0.06163700
H	-8.97732100	2.06096600	-0.96816500
H	-6.25804300	-0.66027700	0.98127700
N	-8.66552000	-0.43293900	0.17871400
C	-9.97746800	-0.29017100	0.29343700
C	-10.77525100	-1.48310700	0.09341100
C	-10.69029500	0.90886400	0.69582700
C	-12.13277500	-1.46730300	0.14044600
H	-10.22856200	-2.39707700	-0.11939100
C	-12.04461000	0.91422900	0.80013400
H	-10.12058200	1.78960300	0.97114700
C	-12.85653200	-0.24571500	0.46647200
H	-12.69635100	-2.37980300	-0.01892400
H	-12.58343200	1.79687000	1.13150500
N	-14.15726800	-0.09904000	0.56366000
C	-15.07279800	-1.05809400	0.13901400
C	-16.20715700	-1.27855900	0.94795700
C	-14.99113100	-1.72991200	-1.10035600
C	-17.18905900	-2.18404000	0.56177400
H	-16.28286200	-0.73407500	1.88422400

C	-15.99602300	-2.61159000	-1.49301100
H	-14.15932600	-1.51970300	-1.76590600
C	-17.09102300	-2.85577700	-0.66133600
H	-18.04488700	-2.35614000	1.20935900
H	-15.92405600	-3.10797100	-2.45747600
H	-17.86911600	-3.54828200	-0.96993100

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction= 0.749598 (Hartree/Particle)
Thermal correction to Energy= 0.794208
Thermal correction to Enthalpy= 0.795152
Thermal correction to Gibbs Free Energy= 0.672231

Energy at B3LYP/6-311++G(d,p)

HF= -3431.828572

Name of compound	C60-E1 cation

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	2.49829200	-0.32753500	-2.77740600
C	3.45226400	0.71697600	-3.10202300
C	4.76872500	0.38065700	-3.43935800
C	5.18238000	-1.01320800	-3.44866100
C	4.26582800	-2.01651600	-3.13723700
C	2.89479100	-1.66977600	-2.80064600
C	1.61833800	0.16614800	-1.75355200
C	1.82479500	1.67298500	-1.56718700
C	3.16799000	1.86239300	-2.28156200
C	4.20849400	2.60724200	-1.77526100
C	5.85790700	1.17241100	-2.92157500
C	6.53704600	-1.07729600	-2.92835300
C	6.91825700	-2.14206100	-2.11025200
C	5.96203400	-3.18814700	-1.78470300
C	4.66246100	-3.12816300	-2.29040700
C	3.53511200	-3.46386300	-1.43600200
C	2.44541000	-2.56061300	-1.75818400
C	1.62138400	-2.06565900	-0.74196400
C	1.20416600	-0.68074200	-0.74898100
C	1.77246200	2.19551100	-0.05465400
C	1.54592900	1.07321600	0.98824000
C	1.18476200	-0.21372800	0.65747600
C	1.58047400	-1.32726600	1.49159700
C	1.85239500	-2.46618400	0.63436700
C	2.89152800	-3.34226600	0.94468800
C	3.75480400	-3.84677000	-0.11127700
C	5.10503200	-3.91303900	0.41195800
C	6.18796700	-3.58924100	-0.40751500
C	6.95397000	0.27628200	-2.60038800
C	7.67846900	-1.00572900	1.77358200
C	8.10641300	-0.14292700	0.76257700
C	7.68741800	1.24452400	0.76915400
C	6.86347400	1.72254900	1.78993900
C	6.41942500	0.82559300	2.84424300
C	5.86176200	-1.55790400	3.15957700
C	6.13300600	-2.69644900	2.29981400
C	7.25700900	-2.35649100	1.44431400

C	7.28323600	-2.79272700	0.11892000
C	7.73381200	-1.89846100	-0.93388300
C	8.13439400	-0.59846500	-0.61979300
C	7.45209200	1.64742200	-0.60885200
C	6.39227700	2.50037400	-0.91254900
C	5.53006000	2.99386500	0.14538100
C	5.76452100	2.61488800	1.47092100
C	4.64898200	2.27669400	2.32159200
C	5.04788900	1.16935600	3.17590200
C	4.13127200	0.16751700	3.48707200
C	4.54498800	-1.22462600	3.48240200
C	5.07710800	-3.45728600	1.79430600
C	3.70978600	-3.10779900	2.12428100
C	3.44613600	-2.01614300	2.95422500
C	2.35829500	-1.11077300	2.63301500
C	2.77683800	0.23142200	2.95913300
C	2.39208700	1.29174700	2.13188400
C	3.35121800	2.33150600	1.80446600
C	3.11250800	2.76514800	0.45468800
C	4.17835700	3.05788900	-0.36584200
C	7.73567600	0.50822500	-1.46701900
C	5.57661500	2.26180600	-2.09042400
C	6.81790100	-0.51224300	2.83416100
C	-0.57599200	3.24117000	-0.04311900
C	-1.29370900	2.07563400	-0.41886900
C	-2.67217100	2.09010300	-0.50756900
C	-3.40625300	3.26248900	-0.22167800
C	-2.69229700	4.43907400	0.11239600
C	-1.32103700	4.42910600	0.20375700
H	-0.76786300	1.16247800	-0.66411000
H	-3.18443800	1.19823600	-0.84804300
H	-3.23648700	5.35620100	0.32416100
H	-0.79470200	5.33963900	0.47723300
N	0.78013600	3.28995600	0.06578900
H	1.04323400	2.23085700	-2.09959200
H	1.17347300	4.17786800	0.35025700
N	-4.78768500	3.33930100	-0.30669900
H	-5.14973900	4.27693800	-0.44688900
C	-5.75661100	2.35636300	-0.22920300
C	-7.04361300	2.65453800	-0.74016500
C	-5.53272500	1.08925000	0.36360400
C	-8.06243200	1.72921000	-0.67492200
H	-7.21887900	3.61708000	-1.21538300
C	-6.54609400	0.15700800	0.40289000
H	-4.57672800	0.86244400	0.81986200
C	-7.84785800	0.44715100	-0.09213000
H	-9.02834000	1.96096200	-1.11091900
H	-6.38105300	-0.81541500	0.85471300
N	-8.77297600	-0.55324300	-0.06795000
C	-10.06155500	-0.41603600	0.14507000
C	-10.90267200	-1.56513500	-0.15323100
C	-10.70670100	0.74100100	0.74892900
C	-12.24813700	-1.52886100	0.00124300
H	-10.39593000	-2.45557500	-0.51146800

C	-12.04594100	0.75524200	0.95487200
H	-10.09003300	1.57055300	1.07812200
C	-12.90880500	-0.33969100	0.53011600
H	-12.84659000	-2.40709500	-0.21229100
H	-12.54059700	1.59953700	1.42493100
N	-14.19036700	-0.16980800	0.73235300
C	-15.18503400	-1.00093300	0.24535600
C	-16.33075700	-1.15677200	1.05848600
C	-15.17027000	-1.60335200	-1.03555200
C	-17.38527200	-1.95815500	0.64209900
H	-16.34827500	-0.65584600	2.02098400
C	-16.25107900	-2.36917200	-1.45890300
H	-14.34198900	-1.41146800	-1.71021200
C	-17.35113200	-2.56660300	-0.61816500
H	-18.24747400	-2.09389800	1.28827200
H	-16.24166600	-2.80745700	-2.45274000
H	-18.18893800	-3.17075300	-0.95339000
Frequency and Energy at B3LYP/6-31G(d)			
Zero-point correction=			0.764436 (Hartree/Particle)
Thermal correction to Energy=			0.809138
Thermal correction to Enthalpy=			0.810082
Thermal correction to Gibbs Free Energy=			0.687245
Energy at B3LYP/6-311++G(d,p)			
HF= -3432.241443			

Name of compound	C60-E1 anion	
Cartesian Coordinates optimized at B3LYP/6-31G(d)		
C	2.58171000	0.12356000	2.84486300
C	3.57003300	-0.90773300	3.07449900
C	4.89760000	-0.55550700	3.38644200
C	5.27549400	0.84896400	3.44647300
C	4.32261300	1.84295200	3.22511600
C	2.94279400	1.48066100	2.93111200
C	1.67866300	-0.33437100	1.82578900
C	1.91411900	-1.82111100	1.54391900
C	3.28704100	-2.01014500	2.19952000
C	4.32621000	-2.70011300	1.61307400
C	5.98051900	-1.27923800	2.77825900
C	6.61094000	0.98291400	2.88863700
C	6.93744800	2.11203400	2.12154000
C	5.94801900	3.14416000	1.89207800
C	4.66013700	3.01525600	2.43687200
C	3.49728600	3.35960300	1.64352600
C	2.43957900	2.40857700	1.95547000
C	1.58919000	1.95244100	0.93761900
C	1.20404900	0.55483700	0.88478400
C	1.81085400	-2.26606500	0.01239800
C	1.52509600	-1.08870700	-0.95308000
C	1.13811000	0.16785600	-0.53956700
C	1.48148700	1.34197400	-1.31973900
C	1.74775800	2.43852000	-0.41487700
C	2.76082400	3.36932100	-0.71618800
C	3.65127900	3.82470500	0.33260900

C	4.98475100	3.96157900	-0.23123600
C	6.10657600	3.62544700	0.53228800
C	7.04380500	-0.33391900	2.46680100
C	7.57653900	1.20910300	-1.84843300
C	8.06379800	0.30441600	-0.90166100
C	7.67974600	-1.09657500	-0.96621800
C	6.82461200	-1.53374400	-1.98604700
C	6.32342400	-0.59752300	-2.97041400
C	5.70146800	1.78733900	-3.13668600
C	5.97082500	2.88158200	-2.22166400
C	7.13556900	2.52834500	-1.42669600
C	7.20145200	2.89126300	-0.08028200
C	7.71252100	1.95215500	0.90435400
C	8.13303000	0.68247000	0.49968900
C	7.51679300	-1.58397700	0.38761100
C	6.47898600	-2.48912900	0.68402700
C	5.58831000	-2.93461900	-0.36514700
C	5.75798200	-2.47537600	-1.67802200
C	4.60694800	-2.13124800	-2.46939800
C	4.94611300	-0.95906400	-3.26257700
C	3.99318200	0.03392300	-3.48257500
C	4.37173600	1.43474000	-3.42369600
C	4.91586600	3.58333400	-1.63181200
C	3.53993800	3.21532100	-1.92697900
C	3.27871700	2.15909000	-2.80874200
C	2.22217100	1.20590900	-2.50111900
C	2.65457800	-0.10018300	-2.92156400
C	2.32950000	-1.22041800	-2.13763300
C	3.32385400	-2.24778300	-1.90527800
C	3.15021800	-2.75744000	-0.57508000
C	4.25375100	-3.07336200	0.18819800
C	7.79179500	-0.48698500	1.29354100
C	5.70115100	-2.33110000	1.89347500
C	6.69038600	0.75640000	-2.90658000
C	-0.52752700	-3.32202400	-0.00968700
C	-1.22957100	-2.24875300	0.56924700
C	-2.61749100	-2.28364400	0.69546200
C	-3.36451700	-3.36903600	0.21995700
C	-2.66850000	-4.43637500	-0.36961300
C	-1.28536000	-4.41901900	-0.47092500
H	-0.70209800	-1.37934200	0.94116800
H	-3.12041800	-1.45630300	1.18542200
H	-3.22399300	-5.28798500	-0.75713900
H	-0.77281600	-5.26600400	-0.92287900
N	0.86171100	-3.39431000	-0.10122300
H	1.16896500	-2.43365800	2.06774900
H	1.18151200	-4.09180500	-0.76047700
N	-4.76552100	-3.46393400	0.36497700
H	-5.11913600	-4.39277800	0.54636200
C	-5.72865200	-2.47088400	0.28646000
C	-7.02982700	-2.75062800	0.75812200
C	-5.48405300	-1.18950800	-0.25360000
C	-8.04950000	-1.81858100	0.66083200
H	-7.22696900	-3.71462100	1.22424500

C	-6.49724800	-0.24700200	-0.30646200
H	-4.49915700	-0.94327300	-0.63377000
C	-7.81965100	-0.53317000	0.10906400
H	-9.02358100	-2.05714700	1.07552300
H	-6.29916900	0.74152300	-0.70983900
N	-8.73939400	0.49446600	0.04087600
C	-10.03247400	0.33329500	-0.15119800
C	-10.86346900	1.51291900	0.02061900
C	-10.72467900	-0.87034700	-0.59133300
C	-12.21664200	1.48229400	-0.08724100
H	-10.33867900	2.43154100	0.26844100
C	-12.07289900	-0.89077800	-0.74932000
H	-10.13705400	-1.74432300	-0.85040600
C	-12.91745200	0.25608000	-0.44854300
H	-12.79669200	2.38732700	0.05852700
H	-12.58519700	-1.77794100	-1.11133600
N	-14.21179600	0.09879600	-0.60231200
C	-15.14866500	1.05406800	-0.22297400
C	-16.23066900	1.30381800	-1.09444800
C	-15.14998600	1.70020400	1.03370600
C	-17.23932900	2.19602200	-0.74627600
H	-16.24637300	0.78639100	-2.04927900
C	-16.17689100	2.57488100	1.38380300
H	-14.35564000	1.48095900	1.74113000
C	-17.22180200	2.83938000	0.49563800
H	-18.05263400	2.38356500	-1.44374900
H	-16.16047700	3.05175800	2.36134700
H	-18.01792600	3.52580500	0.77147700

Frequency and Energy at B3LYP/6-31G(d)
Zero-point correction= 0.759222 (Hartree/Particle) Thermal correction to Energy= 0.804524 Thermal correction to Enthalpy= 0.805468 Thermal correction to Gibbs Free Energy= 0.681066
Energy at B3LYP/6-311++G(d,p)
HF= -3432.564332

Name of compound	C60-L1

Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	2.17359000	-0.86001600	-2.51988300
C	3.15596700	-0.01740900	-3.17691500
C	4.40288300	-0.54565200	-3.53471200
C	4.71787200	-1.93222900	-3.22884300
C	3.77352600	-2.74102600	-2.59786700
C	2.47142800	-2.20001400	-2.24378900
C	1.44340300	-0.05192100	-1.58204700
C	1.76618500	1.42897300	-1.79664400
C	3.03505300	1.31429500	-2.64772800
C	4.17199900	2.06105300	-2.43725100
C	5.59134800	0.24454700	-3.32637000
C	6.11230700	-1.99193300	-2.82565300
C	6.50579000	-2.85748600	-1.80303200
C	5.52069200	-3.70127400	-1.14560000
C	4.18159100	-3.64561800	-1.53687900

C	3.12954500	-3.65957800	-0.53273100
C	2.07574100	-2.76578300	-0.97739600
C	1.40140800	-1.96313900	-0.05049400
C	1.08063100	-0.58958400	-0.36640600
C	1.89689000	2.31685400	-0.47172900
C	1.71942600	1.49161800	0.83132400
C	1.23265100	0.20452300	0.87507700
C	1.64248100	-0.70503100	1.92266100
C	1.74737200	-2.03796600	1.35768700
C	2.75011000	-2.90616900	1.78880700
C	3.46113000	-3.72832100	0.82234500
C	4.85159900	-3.78803800	1.22746800
C	5.86203000	-3.77407900	0.26385300
C	6.65195100	-0.64296300	-2.88428800
C	7.74535100	-0.88616700	1.59345900
C	8.12175400	-0.33717200	0.36551600
C	7.80115900	1.04304200	0.05983800
C	7.12172900	1.82770600	0.99440900
C	6.73112800	1.25725800	2.27337700
C	6.05139800	-0.91689500	3.22325800
C	6.15339600	-2.25032100	2.65706500
C	7.20120700	-2.23216100	1.65029500
C	7.05781800	-2.97721100	0.47873500
C	7.45477000	-2.41049100	-0.79891900
C	7.97372200	-1.11529900	-0.85627000
C	7.44985500	1.11934600	-1.34974800
C	6.42112900	1.96485000	-1.76440300
C	5.71036700	2.77827100	-0.79499100
C	6.05941800	2.71499100	0.55804700
C	5.01828200	2.69549100	1.55686700
C	5.42850300	1.79599700	2.62343800
C	4.48379100	0.98775400	3.25260400
C	4.80076600	-0.39567900	3.56195000
C	5.00015900	-3.00973800	2.44891100
C	3.70150600	-2.46837600	2.79773100
C	3.60060300	-1.18730600	3.34573000
C	2.54710700	-0.29120500	2.90546200
C	3.08779800	1.04548000	2.84550000
C	2.69134900	1.90004500	1.81042700
C	3.67953600	2.73726500	1.15192800
C	3.32715600	2.84814400	-0.23702900
C	4.32024500	2.84400700	-1.18948200
C	7.56339200	-0.21525200	-1.91650300
C	5.47192100	1.52396800	-2.77137000
C	7.03643300	-0.07360300	2.56585400
C	-0.38649200	3.46574800	-0.45385300
C	-1.17758800	2.31735500	-0.59987800
C	-2.56905800	2.38360200	-0.51643800
C	-3.22557100	3.59387000	-0.25932900
C	-2.43204900	4.74503200	-0.10764600
C	-1.04993900	4.68366500	-0.21441200
H	-0.72824500	1.35166400	-0.79359700
H	-3.14596300	1.47723600	-0.66431000
H	-2.91013100	5.69911800	0.10291700

H	-0.46768200	5.59634000	-0.10254400
N	1.01664400	3.48946900	-0.59162800
H	0.97439300	1.91352200	-2.38158500
H	1.42743500	4.31042100	-0.16443000
N	-4.62272900	3.71456700	-0.17434000
H	-5.00148000	4.58299800	-0.52470700
C	-5.56053900	2.69078900	0.02647700
C	-6.81404300	2.75859800	-0.60132300
C	-5.32056700	1.61169300	0.89453100
C	-7.79366000	1.79444200	-0.38004400
H	-7.01968000	3.57262600	-1.29356300
C	-6.29758600	0.64849400	1.11574700
H	-4.37462400	1.54351200	1.42134300
C	-7.55298400	0.71576700	0.48694300
H	-8.73521200	1.86192400	-0.91379000
H	-6.09250400	-0.16663400	1.80677000
N	-8.47636900	-0.31496300	0.70629600
H	-8.07866200	-1.19261200	1.00841800
C	-9.87417100	-0.28331600	0.64663700
C	-10.57292800	-1.49508800	0.50409400
C	-10.62893000	0.89505300	0.77485800
C	-11.96217800	-1.53750200	0.49316000
H	-10.01326500	-2.42417700	0.41671600
C	-12.01847700	0.85566800	0.71698600
H	-10.12950900	1.84506800	0.92834600
C	-12.71546000	-0.35464800	0.57637500
H	-12.46533900	-2.49588600	0.42625300
H	-12.57844600	1.78506700	0.79710100
N	-14.12003800	-0.34066800	0.59181100
H	-14.53989000	0.41076500	1.12009200
C	-15.01954000	-1.21890600	-0.01338800
C	-16.34849000	-1.24557500	0.45186700
C	-14.67164700	-2.04817700	-1.09561900
C	-17.29413700	-2.07531400	-0.14228500
H	-16.63035500	-0.61137900	1.29025500
C	-15.62602400	-2.88491800	-1.67198900
H	-13.66513500	-2.01842800	-1.49746900
C	-16.94113000	-2.91048300	-1.20506900
H	-18.31319500	-2.07443500	0.23639800
H	-15.33455800	-3.51565800	-2.50830400
H	-17.67745400	-3.56522500	-1.66162100

Frequency and Energy at B3LYP/6-31G(d)
Zero-point correction= 0.786904 (Hartree/Particle) Thermal correction to Energy= 0.832982 Thermal correction to Enthalpy= 0.833926 Thermal correction to Gibbs Free Energy= 0.707521
Energy at B3LYP/6-311++G(d,p)
HF= -3433.712117

Name of compound	C60-L1-N1-H radical

Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	2.11431500	-0.97298300	-2.43864900
C	3.05793500	-0.12867900	-3.14833300

C	4.30523100	-0.64134700	-3.52833500
C	4.65943500	-2.01119000	-3.19211100
C	3.75201100	-2.82231100	-2.51196800
C	2.44970100	-2.29822000	-2.13405600
C	1.39105700	-0.15370900	-1.50418000
C	1.67234100	1.32773100	-1.77367400
C	2.92051000	1.21552700	-2.65606300
C	4.04803600	1.98906400	-2.49339700
C	5.48119300	0.17928800	-3.37676900
C	6.06618500	-2.03007800	-2.82927200
C	6.50819900	-2.85756200	-1.79494500
C	5.56151900	-3.70289800	-1.08522000
C	4.21064500	-3.68666300	-1.43809800
C	3.18888300	-3.69432700	-0.40316300
C	2.10340900	-2.83598400	-0.84111800
C	1.43792200	-2.02179700	0.08219800
C	1.07740400	-0.66479500	-0.26314700
C	1.81996300	2.26037500	-0.47035500
C	1.70528900	1.46379000	0.85689700
C	1.24904100	0.16762800	0.95115100
C	1.70890500	-0.70247200	2.01092200
C	1.82704100	-2.04852000	1.48076600
C	2.86050300	-2.88292900	1.90660600
C	3.56107300	-3.71724100	0.94298700
C	4.96381000	-3.73600600	1.30840300
C	5.94514700	-3.72772100	0.31511100
C	6.57404000	-0.67221600	-2.94214000
C	7.80278900	-0.76319200	1.50627500
C	8.13076500	-0.24147400	0.25285800
C	7.77281600	1.12298400	-0.08235700
C	7.10147300	1.91932300	0.84876900
C	6.76084400	1.37696900	2.15453200
C	6.15733400	-0.78288800	3.18547700
C	6.27207300	-2.12937200	2.65412700
C	7.28995200	-2.11819300	1.61678300
C	7.12936700	-2.90027700	0.47178700
C	7.47581800	-2.36174500	-0.83239900
C	7.96363500	-1.05769000	-0.94136000
C	7.37738800	1.15047500	-1.48145000
C	6.31753000	1.96130500	-1.88823000
C	5.61775900	2.78826100	-0.92232300
C	6.00993200	2.77375100	0.42061900
C	4.99740200	2.75787400	1.44856700
C	5.45725400	1.89784600	2.52713900
C	4.54937000	1.08829000	3.20750000
C	4.90576700	-0.27861300	3.54599900
C	5.13056400	-2.91946600	2.50235600
C	3.83106900	-2.39587500	2.87394000
C	3.71765000	-1.10182300	3.38807000
C	2.63243400	-0.24111500	2.95432500
C	3.14182500	1.10429400	2.84005400
C	2.69839400	1.92031400	1.79237400
C	3.64689100	2.75970600	1.08127000
C	3.25189800	2.81483800	-0.29691100

C	4.21571900	2.81620200	-1.27695400
C	7.50314700	-0.19734100	-2.01376800
C	5.34887600	1.47042000	-2.85249600
C	7.10399200	0.06194400	2.47548300
C	-0.38681100	3.34717600	-0.51858300
C	-1.21864300	2.17871800	-0.42568900
C	-2.59460300	2.26551600	-0.38366500
C	-3.25033400	3.51961300	-0.42900000
C	-2.45254500	4.68798000	-0.55563700
C	-1.08435100	4.60421800	-0.60047500
H	-0.77048700	1.19427700	-0.40437200
H	-3.18513500	1.35679200	-0.34073100
H	-2.94080300	5.65967100	-0.60144900
H	-0.47269400	5.49669800	-0.68562700
N	0.94764500	3.43264300	-0.55675000
H	0.85040800	1.77200400	-2.34957100
N	-4.62262000	3.65188100	-0.39656600
H	-4.97993700	4.55776800	-0.66966500
C	-5.59310100	2.70901000	0.00765200
C	-6.83351900	2.67790800	-0.64412100
C	-5.38647300	1.83452600	1.08612200
C	-7.84058700	1.80673600	-0.24274200
H	-7.00594800	3.33353900	-1.49449900
C	-6.38629100	0.95766500	1.48434400
H	-4.45030400	1.86267300	1.63365100
C	-7.63516200	0.92366900	0.83357700
H	-8.77607600	1.78671600	-0.78949400
H	-6.20999400	0.30055400	2.33304400
N	-8.58800700	0.00356700	1.26296600
H	-8.22713700	-0.77590100	1.79453400
C	-9.96504000	-0.04448600	0.98322500
C	-10.60339400	-1.29209700	0.90735800
C	-10.75498700	1.10818600	0.84365000
C	-11.97457300	-1.39534900	0.69932100
H	-10.01548600	-2.19943600	1.02806600
C	-12.11781100	1.00511600	0.58843300
H	-10.30417600	2.08975800	0.94355700
C	-12.75785500	-0.24385200	0.51051000
H	-12.43966700	-2.37456300	0.69073200
H	-12.70468800	1.91230700	0.46183700
N	-14.14346000	-0.28256700	0.31172900
H	-14.64716400	0.53558900	0.62344300
C	-14.93657400	-1.30240500	-0.22321000
C	-16.30777800	-1.32043500	0.09269400
C	-14.43585800	-2.27924400	-1.10228700
C	-17.14930200	-2.28699100	-0.44970000
H	-16.70634100	-0.57140400	0.77409000
C	-15.28680500	-3.25157700	-1.62580200
H	-13.39184100	-2.26067700	-1.39427400
C	-16.64549200	-3.26788900	-1.30707000
H	-18.20495000	-2.27763900	-0.19075200
H	-14.87914500	-3.99658500	-2.30450300
H	-17.30082400	-4.02799700	-1.72175200

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction=	0.774128 (Hartree/Particle)
Thermal correction to Energy=	0.819763
Thermal correction to Enthalpy=	0.820707
Thermal correction to Gibbs Free Energy=	0.695452
Energy at B3LYP/6-311++G(d,p)	
HF= -3433.073514	

Name of compound	C60-L1-N2-H radical		
Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	-2.21008000	-0.87698300	2.54481400
C	-3.17632100	-0.00255500	3.18401500
C	-4.43946600	-0.49470400	3.53612200
C	-4.78714200	-1.87590500	3.24197000
C	-3.85840900	-2.71525400	2.62813600
C	-2.53964700	-2.21194600	2.28017400
C	-1.45157500	-0.09808800	1.60473000
C	-1.73840200	1.39275600	1.80095600
C	-3.01716900	1.31975300	2.64157300
C	-4.13268400	2.09295600	2.41293000
C	-5.60540200	0.32327800	3.30868800
C	-6.17917500	-1.90448900	2.82734800
C	-6.58593100	-2.77084400	1.81062500
C	-5.61714100	-3.64637600	1.17089700
C	-4.28044600	-3.62057300	1.57329500
C	-3.22066500	-3.67223300	0.57872700
C	-2.14768300	-2.80136000	1.02324100
C	-1.44549900	-2.02598700	0.09378800
C	-1.09243500	-0.65768500	0.39816100
C	-1.83659100	2.26830900	0.46403600
C	-1.66811400	1.42578800	-0.82847500
C	-1.21439100	0.12646600	-0.85289400
C	-1.63775000	-0.78361200	-1.89467600
C	-1.78126500	-2.10730300	-1.31652600
C	-2.80217700	-2.95424300	-1.74729600
C	-3.54233200	-3.74729600	-0.77835700
C	-4.93033400	-3.77616800	-1.19514900
C	-5.94834300	-3.72589300	-0.24061700
C	-6.68446200	-0.54166900	2.86674000
C	-7.74556700	-0.80545200	-1.61740600
C	-8.11828300	-0.23380800	-0.39877300
C	-7.76509400	1.14100300	-0.10499500
C	-7.05855100	1.89827600	-1.04205300
C	-6.67177000	1.30417000	-2.31153600
C	-6.03933100	-0.89703100	-3.23195600
C	-6.17996300	-2.22112100	-2.65218800
C	-7.23543500	-2.16530700	-1.65500600
C	-7.12154000	-2.90128800	-0.47450600
C	-7.51460400	-2.31070400	0.79355200
C	-8.00049200	-1.00216300	0.83246700
C	-7.42415700	1.22376000	1.30678700
C	-6.37787700	2.04724300	1.72158700
C	-5.63831500	2.83145200	0.74961600
C	-5.97703100	2.76211600	-0.60568500

C	-4.92854500	2.70550500	-1.59531600
C	-5.35264700	1.80526300	-2.65573100
C	-4.42356400	0.96644000	-3.26769700
C	-4.77296200	-0.41168800	-3.56530900
C	-5.04846600	-3.00751300	-2.42589100
C	-3.73344900	-2.50340000	-2.76918600
C	-3.59545100	-1.23124200	-3.32971600
C	-2.52346000	-0.35751000	-2.88938500
C	-3.03014200	0.99307100	-2.84892200
C	-2.62080800	1.84887800	-1.82006200
C	-3.59268900	2.71796500	-1.17955000
C	-3.24969600	2.83563800	0.21119700
C	-4.25031900	2.86538000	1.15541300
C	-7.57655600	-0.10138300	1.88664800
C	-5.44884500	1.59329600	2.74151700
C	-7.00818700	-0.02178400	-2.59229500
C	0.46877000	3.38179700	0.47783200
C	1.24022600	2.21514600	0.63708100
C	2.62717000	2.26343100	0.57655800
C	3.32827100	3.48101100	0.36895600
C	2.53167600	4.65508700	0.25883300
C	1.15352800	4.60541500	0.28913400
H	0.76650500	1.25822900	0.81775200
H	3.18667900	1.34968000	0.74589200
H	3.04778300	5.60135300	0.12864100
H	0.57842200	5.52376900	0.18478700
N	-0.92431900	3.41624900	0.56457700
H	-0.93860500	1.86189300	2.38750700
H	-1.33031200	4.27584000	0.21950100
N	4.68460200	3.64791500	0.36727300
C	5.55659800	2.65764200	0.03513000
C	6.89509800	2.79108600	0.50230300
C	5.29040600	1.53655700	-0.80645000
C	7.87663400	1.86125400	0.21703500
H	7.11650500	3.64423400	1.13629400
C	6.28096800	0.62772800	-1.12590800
H	4.30846300	1.42707700	-1.25398000
C	7.59129400	0.75332500	-0.61234500
H	8.86499500	1.97397700	0.64782600
H	6.05697700	-0.19540400	-1.80233800
N	8.52148700	-0.22821500	-0.92891700
H	8.13072800	-1.09524400	-1.27116200
C	9.92041300	-0.21346400	-0.80115400
C	10.59344500	-1.42282300	-0.56492700
C	10.69188400	0.94863900	-0.96621800
C	11.98032300	-1.47940700	-0.48859000
H	10.01794800	-2.33889200	-0.45032800
C	12.07591400	0.89989300	-0.84619000
H	10.20941700	1.89129500	-1.19951900
C	12.75058200	-0.30927300	-0.60426700
H	12.46763700	-2.43733100	-0.34671500
H	12.65073000	1.81679400	-0.95708100
N	14.14977400	-0.30475300	-0.55335900
H	14.59755500	0.44591500	-1.05958900

C	15.01921000	-1.20329300	0.07262700
C	16.34800300	-1.27903300	-0.38449100
C	14.63903400	-1.99657800	1.16994500
C	17.26493000	-2.12398000	0.23346400
H	16.65308000	-0.67230800	-1.23477000
C	15.56339700	-2.85068100	1.76954300
H	13.63286300	-1.92399000	1.56733000
C	16.87943800	-2.92525500	1.31072500
H	18.28576700	-2.16233400	-0.13800900
H	15.24881200	-3.45364100	2.61769600
H	17.59294800	-3.59184500	1.78591600

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction=	0.774411 (Hartree/Particle)
Thermal correction to Energy=	0.819869
Thermal correction to Enthalpy=	0.820813
Thermal correction to Gibbs Free Energy=	0.695645

Energy at B3LYP/6-311++G(d,p)

HF= -3433.079528

Name of compound	C60-L1-N3-H radical

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	2.54552900	-0.44425300	-2.82711400
C	3.55224100	0.53351500	-3.19875400
C	4.85977600	0.11834400	-3.48230800
C	5.21067300	-1.28926900	-3.38450000
C	4.24357600	-2.22777000	-3.02766000
C	2.88135300	-1.80143400	-2.75183000
C	1.66633500	0.15939400	-1.86280300
C	1.93371400	1.66430000	-1.77326100
C	3.29896800	1.74379300	-2.46499900
C	4.36107700	2.47797500	-1.98787900
C	5.97113500	0.89646600	-2.99254200
C	6.54875400	-1.37528900	-2.82569000
C	6.86501200	-2.39690700	-1.92816400
C	5.85633500	-3.37604200	-1.55618900
C	4.57173300	-3.29390000	-2.09669700
C	3.41115900	-3.52122000	-1.25083300
C	2.37014200	-2.59724000	-1.66272400
C	1.54835200	-1.99567000	-0.70315400
C	1.19337700	-0.59842300	-0.81380200
C	1.86163900	2.30262800	-0.30771900
C	1.57452400	1.25442800	0.79884500
C	1.15651100	-0.03462500	0.55574100
C	1.48735400	-1.10353200	1.47260500
C	1.73023300	-2.30972100	0.70265500
C	2.71996700	-3.20846400	1.09962700
C	3.58348700	-3.82134900	0.10235800
C	4.91784300	-3.90837800	0.66247800
C	6.03284100	-3.68930700	-0.14935600
C	7.01829300	-0.02112100	-2.58124900
C	7.58763300	-1.02639400	1.88699500
C	8.07605400	-0.25457000	0.83024700
C	7.72038400	1.14739600	0.73110600

C	6.89382600	1.72966700	1.69469400
C	6.38629300	0.92718900	2.79587500
C	5.71744800	-1.40272600	3.26136000
C	5.95684700	-2.60876900	2.48872800
C	7.11380500	-2.37754400	1.64047300
C	7.15029300	-2.90553700	0.34895700
C	7.66366900	-2.10655400	-0.75080200
C	8.11472600	-0.80585200	-0.51660600
C	7.53374900	1.46311000	-0.67659900
C	6.51758300	2.33573700	-1.06469600
C	5.65485100	2.93960400	-0.06582000
C	5.84397800	2.64552200	1.28865900
C	4.69520800	2.41402100	2.13016900
C	5.02440800	1.35203600	3.06777000
C	4.05705300	0.41426200	3.42264900
C	4.40902800	-0.99093300	3.52442200
C	4.87915000	-3.35641200	2.00942500
C	3.52096800	-2.92792000	2.28060900
C	3.28719900	-1.76935600	3.02512700
C	2.24675600	-0.84324800	2.61760500
C	2.71796300	0.49905200	2.85948900
C	2.40079500	1.51236100	1.94817900
C	3.41346300	2.48451800	1.57423300
C	3.22292000	2.82968600	0.19227000
C	4.31933600	3.02966100	-0.61452600
C	7.78533900	0.25570900	-1.44742100
C	5.71865000	2.05190200	-2.24418000
C	6.72620600	-0.42384700	2.88897000
C	-0.46444800	3.36379800	-0.29178600
C	-1.19495300	2.25494900	-0.74723400
C	-2.58940900	2.26436000	-0.74994000
C	-3.30803500	3.36907100	-0.27363300
C	-2.57787500	4.47978700	0.18165200
C	-1.19086200	4.48011800	0.16418100
H	-0.69139000	1.37324900	-1.12395700
H	-3.11971800	1.40567700	-1.14678100
H	-3.10811000	5.34912900	0.56384100
H	-0.65488700	5.35764400	0.52035900
N	0.93804300	3.45132300	-0.32224900
H	1.19283200	2.22296900	-2.35893500
H	1.28519300	4.21679900	0.24195600
N	-4.71232700	3.43620600	-0.28487800
H	-5.09926100	4.35921900	-0.42451700
C	-5.64654200	2.41930200	-0.13437100
C	-6.97937100	2.66313700	-0.53383700
C	-5.34023000	1.15726400	0.42245200
C	-7.96898000	1.71298700	-0.36501500
H	-7.22309200	3.61449100	-1.00385900
C	-6.32289400	0.19506500	0.55466400
H	-4.33238600	0.94669700	0.76211900
C	-7.68057000	0.43412100	0.19763600
H	-8.96973100	1.92371900	-0.72632100
H	-6.08470300	-0.77690500	0.97576000
N	-8.54810700	-0.60370700	0.34603800

C	-9.90112000	-0.44847000	0.43597800
C	-10.69954000	-1.58109300	0.11703900
C	-10.59426300	0.69743000	0.92101300
C	-12.07983200	-1.55986900	0.19480200
H	-10.18165600	-2.48141000	-0.19946400
C	-11.97495700	0.71365000	1.01757300
H	-10.03021200	1.55806600	1.26411500
C	-12.75221500	-0.39844800	0.63317400
H	-12.64578600	-2.45323400	-0.04396700
H	-12.47577300	1.60184300	1.39946000
N	-14.13701300	-0.32450500	0.77647000
H	-14.46458300	0.38061100	1.42217300
C	-15.14447600	-1.07061800	0.15348000
C	-16.39773400	-1.15990000	0.78653300
C	-14.97550200	-1.68552100	-1.09971200
C	-17.44772000	-1.84896800	0.18703400
H	-16.53764100	-0.68990700	1.75784800
C	-16.03058700	-2.38638500	-1.68152500
H	-14.03252300	-1.59147200	-1.62608100
C	-17.27130100	-2.47666100	-1.04833400
H	-18.40693800	-1.90306800	0.69535800
H	-15.88023200	-2.85358300	-2.65145400
H	-18.08816000	-3.02261600	-1.51089900
Frequency and Energy at B3LYP/6-31G(d)			
Zero-point correction=			0.774657 (Hartree/Particle)
Thermal correction to Energy=			0.819982
Thermal correction to Enthalpy=			0.820927
Thermal correction to Gibbs Free Energy=			0.696781
Energy at B3LYP/6-311++G(d,p)			
HF= -3433.079373			

Name of compound	C60-L1-N4-H radical	
Cartesian Coordinates optimized at B3LYP/6-31G(d)		
C	-2.51499900	-0.34826000	2.81664900
C	-3.53622400	0.62345400	3.16346800
C	-4.83603100	0.19560800	3.46272800
C	-5.16464400	-1.21963900	3.40644500
C	-4.18356400	-2.15248900	3.07364300
C	-2.82917200	-1.71226700	2.78124100
C	-1.64804800	0.24185100	1.83310500
C	-1.94002400	1.73923700	1.70162500
C	-3.30441300	1.81629900	2.39496000
C	-4.37946200	2.51946100	1.90063900
C	-5.96095200	0.94175800	2.95486800
C	-6.50274900	-1.34270200	2.85466500
C	-6.80543400	-2.39441600	1.98773900
C	-5.78187700	-3.36715700	1.64030900
C	-4.49727800	-3.24973100	2.17445000
C	-3.33546700	-3.48271600	1.33155200
C	-2.30845300	-2.53047700	1.71346200
C	-1.49892800	-1.94330500	0.73465300
C	-1.16578500	-0.53802100	0.80450200
C	-1.88148400	2.33667800	0.21857000

C	-1.58149700	1.26163500	-0.85842800
C	-1.14131100	-0.01299600	-0.58066600
C	-1.45801400	-1.11258900	-1.46583500
C	-1.67936100	-2.30018600	-0.66116700
C	-2.65581200	-3.22554900	-1.02919100
C	-3.50686500	-3.82352000	-0.01220700
C	-4.84119000	-3.94708700	-0.56533700
C	-5.95724400	-3.72288700	0.24353300
C	-6.99442400	-0.00363200	2.57333600
C	-7.56021800	-1.14418600	-1.86269000
C	-8.05783400	-0.35055000	-0.82656600
C	-7.72422200	1.05908800	-0.76830900
C	-6.90975200	1.62694700	-1.75055600
C	-6.39261200	0.80167900	-2.83018700
C	-5.68788100	-1.52950300	-3.23141800
C	-5.90592900	-2.71691000	-2.42434300
C	-7.06414600	-2.48004300	-1.57933700
C	-7.08867200	-2.97178900	-0.27326500
C	-7.61172900	-2.15018800	0.80501400
C	-8.08405700	-0.86394200	0.53548900
C	-7.53904500	1.41771000	0.62925900
C	-6.53596500	2.31726700	0.98904000
C	-5.68552000	2.90620700	-0.02926500
C	-5.87380700	2.57102200	-1.37434700
C	-4.72370300	2.33380600	-2.21258100
C	-5.03849900	1.24039300	-3.11846100
C	-4.05724000	0.30839700	-3.44964500
C	-4.38703400	-1.10448500	-3.50996800
C	-4.81498100	-3.43317700	-1.92737100
C	-3.46456500	-2.99133000	-2.21512100
C	-3.25161700	-1.85057200	-2.99256800
C	-2.22489900	-0.89695000	-2.61507000
C	-2.71815800	0.43030500	-2.89338800
C	-2.41463500	1.47392500	-2.01214000
C	-3.44173100	2.44020400	-1.66269900
C	-3.25261700	2.82760600	-0.29178900
C	-4.35007700	3.03256200	0.51230800
C	-7.76892100	0.22876100	1.43481600
C	-5.72923600	2.07947600	2.17347100
C	-6.71115000	-0.55665600	-2.88385900
C	0.42991500	3.42734400	0.17922500
C	1.17175100	2.34639100	0.67940400
C	2.56634700	2.37612300	0.69507500
C	3.27566000	3.47265700	0.18735800
C	2.53319200	4.55309800	-0.31853000
C	1.14578900	4.53463500	-0.31248900
H	0.67795500	1.47048600	1.08168900
H	3.10333100	1.53808700	1.12603100
H	3.05437700	5.41542100	-0.72821100
H	0.60175700	5.39118700	-0.70575800
N	-0.97580300	3.49908700	0.19842800
H	-1.20721000	2.32641500	2.26921200
H	-1.32604500	4.23154100	-0.40659200
N	4.67767300	3.56179500	0.21158900

H	5.05204400	4.49540800	0.30059800
C	5.62526000	2.53921700	0.16386000
C	6.92720200	2.79583700	0.63225300
C	5.35901700	1.26578900	-0.37119200
C	7.92270600	1.82833700	0.57646400
H	7.15362400	3.76547700	1.07055600
C	6.35914000	0.30161200	-0.43240400
H	4.37739100	1.04018800	-0.77210400
C	7.65575900	0.56018100	0.03619500
H	8.90337100	2.04828700	0.98433000
H	6.13508000	-0.66768000	-0.87221800
N	8.61397200	-0.47187700	0.00569900
H	8.24819000	-1.40578100	0.13227300
C	9.98283300	-0.39288100	-0.18359200
C	10.77293400	-1.52977000	0.11161000
C	10.62939000	0.74971500	-0.71370800
C	12.14124500	-1.52080200	-0.05921400
H	10.28298400	-2.42978700	0.47996100
C	11.99503200	0.75199600	-0.90220600
H	10.04258000	1.61333100	-1.00546900
C	12.82074400	-0.36061700	-0.55200900
H	12.70895200	-2.42091200	0.14889300
H	12.49121300	1.61931600	-1.32688000
N	14.14232100	-0.23971700	-0.79900800
C	15.08890000	-1.08643400	-0.26160800
C	16.25266300	-1.32453300	-1.03350300
C	15.03651000	-1.64525300	1.04112700
C	17.27955400	-2.12725300	-0.55429800
H	16.30655400	-0.87071000	-2.01844500
C	16.08481700	-2.42386300	1.52301100
H	14.19075300	-1.41887500	1.68270600
C	17.20422000	-2.68472500	0.72776500
H	18.15273500	-2.31069500	-1.17552300
H	16.03080900	-2.82629300	2.53184000
H	18.01588800	-3.29880400	1.10799600

Frequency and Energy at B3LYP/6-31G(d)
Zero-point correction= 0.774411 (Hartree/Particle) Thermal correction to Energy= 0.819847 Thermal correction to Enthalpy= 0.820792 Thermal correction to Gibbs Free Energy= 0.696209
Energy at B3LYP/6-311++G(d,p)
HF= -3433.076212

Name of compound	C60-L1 cation

Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	2.46775300	-0.53793300	-2.71401100
C	3.42109800	0.46620900	-3.14935700
C	4.72286900	0.08817700	-3.49968300
C	5.12258500	-1.30711500	-3.41114600
C	4.20662500	-2.27151400	-2.99318800
C	2.85008400	-1.88282200	-2.64365700
C	1.62557900	0.04645500	-1.70613000
C	1.85145900	1.56046400	-1.64562600

C	3.17309900	1.67609300	-2.41364900
C	4.23640900	2.44617800	-2.00095300
C	5.83526100	0.90498600	-3.07995500
C	6.49213400	-1.34627100	-2.92861900
C	6.88890000	-2.34777100	-2.04086700
C	5.93330000	-3.35310300	-1.60430900
C	4.61904500	-3.31734900	-2.07322800
C	3.51581000	-3.57084500	-1.16089200
C	2.42530600	-2.68277400	-1.52049200
C	1.63887800	-2.09849100	-0.52184300
C	1.23481600	-0.71367800	-0.62559400
C	1.84794800	2.20580100	-0.17983100
C	1.64729600	1.16762900	0.95373900
C	1.26198000	-0.13683000	0.73939500
C	1.67433900	-1.18588500	1.64628900
C	1.90870500	-2.39223500	0.87428100
C	2.94837700	-3.25421900	1.22133700
C	3.77319100	-3.85089500	0.18272700
C	5.13854800	-3.89195600	0.66807800
C	6.19838500	-3.64697500	-0.20720800
C	6.93201500	0.02388600	-2.72190000
C	7.78153100	-0.91749100	1.71565300
C	8.18550800	-0.14241000	0.62671100
C	7.78056300	1.24626200	0.53595500
C	6.99340300	1.81324100	1.54013200
C	6.57403300	1.00768700	2.67528000
C	6.00385000	-1.33650200	3.19573500
C	6.23705500	-2.54269500	2.42124800
C	7.33694100	-2.28494100	1.50755100
C	7.31741900	-2.82482200	0.22071900
C	7.74334800	-2.02197600	-0.91297900
C	8.16594200	-0.70603700	-0.71537800
C	7.50624100	1.54204100	-0.86181700
C	6.44501100	2.38067700	-1.19944600
C	5.62119000	2.96670400	-0.15825500
C	5.89388000	2.69127700	1.18541200
C	4.80225000	2.43445300	2.09339700
C	5.21693600	1.39327400	3.02017000
C	4.30075400	0.43038300	3.43777000
C	4.70099500	-0.96261500	3.53058000
C	5.15839000	-3.32829800	2.01022600
C	3.80541000	-2.93740400	2.35308500
C	3.57840300	-1.78003000	3.10095100
C	2.48941900	-0.88994300	2.74309500
C	2.93089000	0.46867500	2.94836100
C	2.53067700	1.46422300	2.05063000
C	3.48952500	2.46297300	1.61254600
C	3.21241800	2.79085600	0.24082700
C	4.25476200	3.00752500	-0.63146000
C	7.75140400	0.33511000	-1.63512300
C	5.59039600	2.05981300	-2.32922900
C	6.95950300	-0.33143400	2.75957100
C	-0.48853600	3.27402700	-0.18965400
C	-1.22466300	2.10009100	-0.47338200

C	-2.60940100	2.12739200	-0.54151100
C	-3.32288300	3.31842400	-0.31684300
C	-2.59304500	4.49762000	-0.05939800
C	-1.21562900	4.47731200	0.00271200
H	-0.71682700	1.16364800	-0.66305600
H	-3.13706300	1.21998200	-0.81288300
H	-3.12222600	5.43203400	0.11145300
H	-0.67625400	5.39774800	0.21092100
N	0.87949000	3.31821100	-0.12061500
H	1.05894800	2.08388600	-2.19617500
H	1.28170600	4.20990400	0.13349500
N	-4.71715400	3.40493000	-0.39793900
H	-5.07108200	4.31486400	-0.66940900
C	-5.68440900	2.45344900	-0.15694600
C	-6.99656100	2.68840600	-0.63459600
C	-5.44303200	1.26500900	0.57304300
C	-8.01809300	1.78967000	-0.40763700
H	-7.19599700	3.57991300	-1.22401600
C	-6.46491000	0.36668000	0.79986500
H	-4.46442700	1.07657500	0.99714900
C	-7.77679700	0.60220200	0.32302800
H	-8.99613200	1.97743300	-0.83353300
H	-6.26539500	-0.52503200	1.38893300
N	-8.74538900	-0.35033400	0.56389100
H	-8.39117100	-1.26468900	0.81989900
C	-10.13842100	-0.25741100	0.51054900
C	-10.87928800	-1.43558800	0.29037700
C	-10.84158800	0.94317100	0.73625700
C	-12.26131400	-1.42141600	0.25286900
H	-10.35539100	-2.37745100	0.14472600
C	-12.22332600	0.96239900	0.69012400
H	-10.30653800	1.85254900	0.98420700
C	-12.97059000	-0.21087600	0.43198800
H	-12.80098000	-2.34870300	0.10550300
H	-12.74750900	1.89761300	0.87070400
N	-14.34551600	-0.13058500	0.42029900
H	-14.73479800	0.71433400	0.81860200
C	-15.29568400	-1.08751400	0.00091900
C	-16.51492600	-1.16126800	0.69187100
C	-15.08174900	-1.91165800	-1.11478500
C	-17.49895800	-2.05630600	0.28072400
H	-16.68158300	-0.52351300	1.55663600
C	-16.06777700	-2.81573200	-1.50670700
H	-14.16712900	-1.82115500	-1.69104400
C	-17.27735400	-2.89509400	-0.81403700
H	-18.43807300	-2.10383400	0.82414100
H	-15.89432600	-3.44738100	-2.37322100
H	-18.04321100	-3.59697400	-1.12922200

Frequency and Energy at B3LYP/6-31G(d)	
Zero-point correction=	0.789202 (Hartree/Particle)
Thermal correction to Energy=	0.834625
Thermal correction to Enthalpy=	0.835569
Thermal correction to Gibbs Free Energy=	0.710935
Energy at B3LYP/6-311++G(d,p)	

HF= -3433.506230

Name of compound	C60-L1 anion

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	-3.05795200	0.79054400	2.89388800
C	-4.04333700	1.81919900	2.64740300
C	-5.41336100	1.54672900	2.84195900
C	-5.83023700	0.21573400	3.26000400
C	-4.87952700	-0.77665200	3.49779300
C	-3.46155600	-0.48767400	3.32769700
C	-1.99831200	0.93994300	1.93605000
C	-2.15079500	2.26690800	1.18632600
C	-3.60316500	2.61283700	1.53570900
C	-4.52213100	3.07009900	0.61502400
C	-6.37021500	2.02657300	1.88426800
C	-7.06842600	-0.11054800	2.57200100
C	-7.30169300	-1.42785600	2.14066400
C	-6.31574300	-2.45694300	2.38731800
C	-5.12139400	-2.14002900	3.05903200
C	-3.86070400	-2.67903100	2.59430700
C	-2.83927900	-1.65327300	2.76452100
C	-1.83058100	-1.50712700	1.79992100
C	-1.40646400	-0.18025500	1.39010500
C	-1.80324900	2.23099800	-0.37296100
C	-1.40131000	0.82553800	-0.88405200
C	-1.11426800	-0.23874600	-0.05584000
C	-1.36332800	-1.60219200	-0.48878600
C	-1.78885900	-2.38197200	0.65099100
C	-2.76928500	-3.38568900	0.49109900
C	-3.82124100	-3.52168100	1.47642400
C	-5.05689500	-3.85315300	0.78233100
C	-6.27399800	-3.32831400	1.22780600
C	-7.39715700	1.00645200	1.71204000
C	-7.29989200	-1.77594700	-1.96697200
C	-7.90428100	-0.63968000	-1.42239200
C	-7.47998900	0.68682400	-1.84444300
C	-6.46697200	0.81461900	-2.80471200
C	-5.84514800	-0.36150800	-3.37306200
C	-5.26556300	-2.67220600	-2.71744000
C	-5.69819400	-3.44540700	-1.56777400
C	-6.96244200	-2.89661200	-1.10486400
C	-7.24353000	-2.83880300	0.26139500
C	-7.87573700	-1.65846700	0.82725500
C	-8.19702800	-0.57971000	-0.00119000
C	-7.51767300	1.56323100	-0.69395900
C	-6.51309600	2.54193700	-0.52732400
C	-5.46088000	2.66816100	-1.50989300
C	-5.43640100	1.83036200	-2.63367800
C	-4.18743600	1.29240700	-3.09904700
C	-4.43036500	-0.07294500	-3.54213100
C	-3.47978900	-1.06406100	-3.30393900
C	-3.89700300	-2.39146100	-2.88762300
C	-4.76439900	-3.91261000	-0.63825400

C	-3.34964600	-3.61825600	-0.81358400
C	-2.93129800	-2.87014900	-1.92230100
C	-1.91054700	-1.84349000	-1.75662700
C	-2.23866600	-0.73638400	-2.61257300
C	-2.01034900	0.57722200	-2.16238100
C	-3.00159900	1.60315900	-2.40586800
C	-3.02269000	2.49359900	-1.28084700
C	-4.22258100	2.99866500	-0.82595100
C	-7.95241800	0.78344000	0.44550000
C	-5.93367000	2.76999700	0.77700400
C	-6.25125800	-1.64391100	-2.96321800
C	0.54390400	3.26448600	-0.37446100
C	1.11904300	2.42759800	0.60145600
C	2.47824300	2.50505300	0.89783700
C	3.32656100	3.38409800	0.21327500
C	2.75984800	4.21270600	-0.76547300
C	1.39991700	4.16480300	-1.04286100
H	0.51097500	1.71755600	1.14760600
H	2.88371900	1.87285200	1.68228200
H	3.39575200	4.90056900	-1.31960900
H	0.98561100	4.82707900	-1.80064400
N	-0.81557300	3.29391100	-0.67385200
H	-1.47959000	3.02643500	1.60803400
H	-1.02011200	3.75799300	-1.54922600
N	4.70334600	3.49685600	0.53003000
H	5.09394100	4.42158300	0.41535800
C	5.64456100	2.46919200	0.57363300
C	6.97124700	2.77601800	0.93601000
C	5.34120400	1.12836800	0.27693600
C	7.94984300	1.79201300	1.00692500
H	7.22798200	3.80269900	1.19048600
C	6.33079900	0.15066300	0.33038000
H	4.33576100	0.85512000	-0.02180300
C	7.64798300	0.45700500	0.69598100
H	8.95301400	2.05584500	1.32792100
H	6.07380200	-0.87474100	0.07248800
N	8.60798800	-0.57463200	0.81575100
H	8.23299400	-1.48082700	1.05921400
C	9.90001700	-0.59710700	0.29194300
C	10.73540200	-1.69229500	0.58898300
C	10.41959700	0.41487600	-0.53480200
C	12.02518100	-1.77978600	0.08046900
H	10.35412100	-2.49562200	1.21629600
C	11.72740800	0.34204900	-1.00659500
H	9.79790500	1.25932500	-0.80960500
C	12.55527800	-0.74947200	-0.71259500
H	12.62641100	-2.65826500	0.29284600
H	12.11152900	1.14849300	-1.62817600
N	13.84936200	-0.82207800	-1.27388200
H	13.95358500	-0.38140100	-2.17688800
C	15.04276800	-1.17402200	-0.64802900
C	16.20472800	-1.29936700	-1.43649600
C	15.14991700	-1.39632600	0.73784300
C	17.42483600	-1.63560700	-0.85976900

H	16.13702000	-1.13444800	-2.51032100
C	16.37772800	-1.74229100	1.29982200
H	14.27780800	-1.27966300	1.37112800
C	17.52506600	-1.86718200	0.51471300
H	18.30412100	-1.72304600	-1.49368500
H	16.43452300	-1.90583600	2.37350400
H	18.47677300	-2.13755500	0.96281900

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction= 0.782574 (Hartree/Particle)
Thermal correction to Energy= 0.829048
Thermal correction to Enthalpy= 0.829992
Thermal correction to Gibbs Free Energy= 0.701535

Energy at B3LYP/6-311++G(d,p)

HF= -3433.810724

Name of compound	C60-L2

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	-0.23431100	-1.64455800	-1.57293000
C	0.54966900	-1.09936300	-2.66556500
C	1.61154500	-1.83780300	-3.20260700
C	1.94037700	-3.14124500	-2.64811200
C	1.18682100	-3.66524500	-1.59837800
C	0.07023200	-2.90933400	-1.05436300
C	-0.62144500	-0.55983900	-0.71262600
C	-0.31046900	0.78019000	-1.38178300
C	0.64788900	0.32360800	-2.48406900
C	1.82610500	0.96330000	-2.79374400
C	2.84233800	-1.16395700	-3.53650500
C	3.38772500	-3.26599400	-2.63756300
C	4.02417600	-3.90752400	-1.57327800
C	3.23843600	-4.45427000	-0.47888100
C	1.84738700	-4.33676000	-0.49225400
C	1.13522100	-3.99419600	0.72838100
C	0.03674000	-3.11451900	0.37301800
C	-0.30153900	-2.04416800	1.20870500
C	-0.64158900	-0.75484400	0.65036100
C	0.22425800	1.94111500	-0.42114400
C	0.41034700	1.46272500	1.04888400
C	-0.09591300	0.28405900	1.55451500
C	0.56074200	-0.39600000	2.64881300
C	0.43768600	-1.82724500	2.43948100
C	1.48372500	-2.68039000	2.79013200
C	1.84475600	-3.78244800	1.91253800
C	3.28914200	-3.90688100	1.92614000
C	3.97391900	-4.23575200	0.75406000
C	3.94572000	-2.04040100	-3.18701700
C	6.28827500	-1.35463200	0.73162500
C	6.31294300	-1.15540200	-0.65059800
C	5.97867500	0.14260300	-1.20278900
C	5.63571500	1.19742800	-0.35374400
C	5.61117900	0.99095000	1.08557400
C	5.14399500	-0.80664800	2.71117900
C	5.01747000	-2.23798700	2.50131000

C	5.72579300	-2.57758300	1.27864500
C	5.21431300	-3.55490300	0.42318100
C	5.24434500	-3.35218900	-1.01548100
C	5.77939800	-2.17510600	-1.54263800
C	5.23420500	-0.07294100	-2.43357800
C	4.16621000	0.76505800	-2.75514100
C	3.80412800	1.85789400	-1.87160900
C	4.53220000	2.07433900	-0.69783000
C	3.82645000	2.40648100	0.51556500
C	4.49115700	1.74232300	1.62502800
C	3.73787600	1.21986700	2.67436800
C	4.07061100	-0.07978600	3.23060300
C	3.82221200	-2.88719400	2.81826800
C	2.70687100	-2.13242400	3.35493400
C	2.82650700	-0.75585400	3.56040800
C	1.73079400	0.12825700	3.20802800
C	2.28825800	1.34093100	2.65979500
C	1.64489800	1.96840100	1.58611700
C	2.43201800	2.50502000	0.49107000
C	1.68914800	2.33724400	-0.72679600
C	2.36329300	1.99335700	-1.87782700
C	5.11810200	-1.50690700	-2.64636900
C	2.94656200	0.21493900	-3.31918200
C	5.93074400	-0.26039300	1.61694300
C	-2.08299800	2.99862200	-0.61134200
C	-2.81248200	2.14197400	0.22446600
C	-4.20386400	2.06414200	0.15300400
C	-4.92189900	2.86001900	-0.75305200
C	-4.19241800	3.73922700	-1.57790900
C	-2.80868400	3.80063700	-1.51058500
H	-2.30066200	1.53430400	0.96066500
H	-4.73196800	1.40660700	0.83446300
H	-4.72351500	4.36335500	-2.29380100
H	-2.26569500	4.47529700	-2.16569600
N	-0.65543200	3.13061800	-0.60278500
H	-1.22370600	1.18141400	-1.83822100
N	-6.31438600	2.85198500	-0.84720800
H	-6.72554500	3.68387400	-1.24571000
C	-7.22576200	1.87490600	-0.41692700
C	-6.92616600	0.50276200	-0.40400200
C	-8.51896000	2.26826700	-0.03534900
C	-7.87246600	-0.43478900	-0.00058100
H	-5.94380000	0.16258900	-0.71316000
C	-9.47795200	1.32849400	0.32226900
H	-8.77650800	3.32512200	-0.02958500
C	-9.17286300	-0.04235600	0.35816800
H	-7.59572500	-1.48265800	0.03697500
H	-10.47920800	1.65980300	0.58868600
N	-10.15100000	-0.94504700	0.80057000
H	-10.83180800	-0.56586500	1.44296400
C	-10.32365600	-2.29255800	0.47459900
C	-11.09273900	-3.09818200	1.33533700
C	-9.80287000	-2.86906100	-0.69800500
C	-11.32933200	-4.43602000	1.03443900

H	-11.49803200	-2.66510900	2.24773400
C	-10.03478900	-4.21458100	-0.97938900
H	-9.24090800	-2.25970100	-1.39688900
C	-10.79551800	-5.01048000	-0.12160200
H	-11.92810200	-5.03532500	1.71564700
H	-9.62382200	-4.63868700	-1.89221000
H	-10.97222300	-6.05722900	-0.35040700
C	-0.17656500	4.40258500	-0.12300100
C	-0.50667700	4.87560400	1.15488500
C	0.61031000	5.21786500	-0.94695400
C	-0.05741200	6.11401400	1.60036600
H	-1.13167800	4.26750800	1.80255800
C	1.07421600	6.45294600	-0.50405700
H	0.86077200	4.87183600	-1.94483900
C	0.74821700	6.92263700	0.77943300
H	-0.33139400	6.46361200	2.59350400
H	1.68267300	7.06921200	-1.16231300
N	1.15781800	8.18909300	1.20430800
H	1.99208600	8.54176100	0.75171800
H	1.20554000	8.30724000	2.20885100

Frequency and Energy at B3LYP/6-31G(d)
Zero-point correction= 0.786238 (Hartree/Particle) Thermal correction to Energy= 0.832367 Thermal correction to Enthalpy= 0.833312 Thermal correction to Gibbs Free Energy= 0.707952
Energy at B3LYP/6-311++G(d,p)
HF= -3433.704021

Name of compound	C60-L2-N1-H radical

Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	-0.06157900	-1.40897400	-1.94133800
C	0.82533800	-0.75545900	-2.88551600
C	1.93668500	-1.44065700	-3.39193900
C	2.21111000	-2.79985000	-2.95433400
C	1.35766200	-3.42847800	-2.04822200
C	0.19196000	-2.72556100	-1.53742500
C	-0.53391000	-0.42168300	-1.00948700
C	-0.15891500	0.98092700	-1.49345300
C	0.90303700	0.63823100	-2.54076300
C	2.10567100	1.29585800	-2.65923000
C	3.19381100	-0.74590500	-3.52666900
C	3.65056300	-2.93844900	-2.81494200
C	4.17963300	-3.69902100	-1.77038700
C	3.28956200	-4.35413800	-0.82533300
C	1.90649600	-4.22325000	-0.96293500
C	1.07656600	-4.00893100	0.21179600
C	0.01751600	-3.08530100	-0.15155000
C	-0.40462400	-2.11028900	0.75958200
C	-0.68862300	-0.76407500	0.31497200
C	0.27865500	2.02189900	-0.36125200
C	0.32025600	1.38451500	1.05608600
C	-0.23457600	0.16364200	1.37582900
C	0.31072000	-0.63743900	2.44897500

C	0.21008700	-2.03585900	2.07299700
C	1.21758000	-2.93176900	2.42914900
C	1.66537400	-3.93451900	1.47600200
C	3.10127500	-4.07350600	1.61851700
C	3.89885600	-4.27885400	0.49088300
C	4.25827500	-1.66544600	-3.16781000
C	6.19989300	-1.43462800	1.01312500
C	6.36178100	-1.08579800	-0.32955700
C	6.08195800	0.26810000	-0.76577700
C	5.65451300	1.22634200	0.15643800
C	5.48761600	0.86416000	1.55463600
C	4.86480800	-1.09594100	2.91893100
C	4.76199700	-2.49448000	2.54150500
C	5.58810900	-2.70500400	1.36455000
C	5.16490800	-3.57764300	0.36063700
C	5.33787000	-3.21948700	-1.03701000
C	5.92148700	-1.99698900	-1.37653000
C	5.46254200	0.19506900	-2.07983900
C	4.43072100	1.07289400	-2.41129700
C	3.98078600	2.06456800	-1.45243400
C	4.58867900	2.14529500	-0.19631800
C	3.76665600	2.35146000	0.97083900
C	4.31934200	1.56342400	2.06053400
C	3.46672900	0.93619200	2.96661200
C	3.74452900	-0.41985800	3.40659000
C	3.54194600	-3.16294600	2.66569000
C	2.37799200	-2.46063900	3.16894000
C	2.47479700	-1.11627100	3.53541200
C	1.41858000	-0.18880500	3.17479300
C	2.02564400	1.07170600	2.82239900
C	1.49099500	1.82105800	1.76728700
C	2.38139400	2.46806800	0.82105600
C	1.76271000	2.44034600	-0.47631100
C	2.54779600	2.21113300	-1.58517800
C	5.37062300	-1.20565400	-2.45950200
C	3.27407400	0.59954100	-3.15047100
C	5.75424300	-0.44071100	1.97350400
C	-2.04588600	3.02630300	-0.58747300
C	-2.82059300	2.19657300	0.23552700
C	-4.19452800	2.06445200	0.04415600
C	-4.84950500	2.77222500	-0.97964000
C	-4.07436800	3.62564700	-1.79196700
C	-2.70652200	3.74505700	-1.59970200
H	-2.35647300	1.65978200	1.05411600
H	-4.76472100	1.43568000	0.71817500
H	-4.55561100	4.18342900	-2.59259200
H	-2.12440300	4.39768900	-2.24379400
N	-0.62846400	3.21206800	-0.45449900
H	-1.02474800	1.43909600	-1.98736000
N	-6.21917800	2.69926200	-1.20607200
H	-6.60863500	3.45972600	-1.74515200
C	-7.15165000	1.76454000	-0.71791700
C	-6.84961500	0.40420500	-0.55077200
C	-8.46132500	2.18721700	-0.44184500

C	-7.81074500	-0.49413900	-0.09580000
H	-5.85362600	0.04025500	-0.77972800
C	-9.43372000	1.28340600	-0.03300400
H	-8.72078800	3.23703800	-0.55834500
C	-9.12744500	-0.07502100	0.16045800
H	-7.53257900	-1.52982300	0.06313100
H	-10.44698400	1.63375700	0.15049100
N	-10.12622300	-0.92834900	0.64443500
H	-10.84980600	-0.48018100	1.18823200
C	-10.24764000	-2.31634100	0.52153200
C	-11.03659200	-3.00513100	1.46127800
C	-9.66021100	-3.04528700	-0.52767600
C	-11.22790400	-4.37956500	1.35686400
H	-11.49348900	-2.45187100	2.27936100
C	-9.84627800	-4.42451400	-0.61107300
H	-9.08414400	-2.53033400	-1.28825400
C	-10.62696800	-5.10431800	0.32505700
H	-11.84341400	-4.88768500	2.09475200
H	-9.38414600	-4.96881100	-1.43079800
H	-10.76818200	-6.17841700	0.25036400
C	-0.23165400	4.47736700	0.05869600
C	-0.90700600	5.04911300	1.16477000
C	0.79398700	5.23127700	-0.56493000
C	-0.55820600	6.29161500	1.64736800
H	-1.70740500	4.48793800	1.63679100
C	1.15094200	6.47327300	-0.08869200
H	1.28001700	4.82893200	-1.44585800
C	0.49590300	7.06317200	1.04598600
H	-1.07807200	6.70441700	2.50960400
H	1.92589500	7.05877200	-0.57355700
N	0.89445300	8.26960800	1.45014900
H	0.33129700	8.55276000	2.26238600

Frequency and Energy at B3LYP/6-31G(d)
Zero-point correction= 0.773414 (Hartree/Particle) Thermal correction to Energy= 0.818985 Thermal correction to Enthalpy= 0.819929 Thermal correction to Gibbs Free Energy= 0.695573
Energy at B3LYP/6-311++G(d,p)
HF= -3433.052621

Name of compound	C60-L2-N3-H radical

Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	-0.38975100	-1.73274300	-1.26731000
C	0.29260600	-1.21992100	-2.44032400
C	1.31336900	-1.96990600	-3.03840500
C	1.69960600	-3.25139800	-2.47003300
C	1.04173100	-3.74441600	-1.34370900
C	-0.03163300	-2.97699300	-0.73386300
C	-0.71272400	-0.62234200	-0.41451000
C	-0.47547600	0.69820300	-1.15185200
C	0.39186900	0.20951500	-2.31601900
C	1.53627000	0.84351400	-2.74199700
C	2.50617600	-1.30044400	-3.49657100

C	3.14393200	-3.36693500	-2.57688500
C	3.87291600	-3.96860500	-1.54919500
C	3.18644700	-4.48228400	-0.37473200
C	1.79827000	-4.37432800	-0.27515100
C	1.18766600	-3.99501400	0.98917600
C	0.05651700	-3.13376200	0.69743700
C	-0.21981800	-2.03808200	1.52256900
C	-0.61461700	-0.77074000	0.95094100
C	0.13043400	1.89506700	-0.27559500
C	0.44037200	1.46974700	1.18966900
C	-0.00735500	0.30277900	1.77145200
C	0.74441600	-0.33603900	2.82894700
C	0.61709000	-1.77440300	2.67883100
C	1.69571200	-2.60919700	2.96948900
C	1.99203700	-3.73818600	2.10184800
C	3.43357700	-3.85302100	1.99802500
C	4.02034900	-4.21677500	0.78419800
C	3.64290200	-2.15730100	-3.21086200
C	6.29914700	-1.32463600	0.47138500
C	6.20598900	-1.17240100	-0.91380900
C	5.81510600	0.10418000	-1.47886400
C	5.53494400	1.18500100	-0.63935200
C	5.63289200	1.02754500	0.80308200
C	5.31964200	-0.71669700	2.52058400
C	5.18913400	-2.15519000	2.37015300
C	5.79538700	-2.53181100	1.10427500
C	5.22256400	-3.54056800	0.32780400
C	5.13037700	-3.38704500	-1.11439200
C	5.60912500	-2.22523400	-1.72349900
C	4.97210500	-0.15801400	-2.63453300
C	3.87360800	0.66182200	-2.89354200
C	3.57669000	1.78053100	-2.01866100
C	4.39869200	2.04252700	-0.91867700
C	3.79393700	2.41141400	0.33825900
C	4.55524000	1.78977700	1.40925800
C	3.89691400	1.29867700	2.53481400
C	4.28706500	0.02094100	3.10413700
C	4.03012800	-2.80024400	2.80765300
C	2.95711800	-2.03459600	3.41068900
C	3.08106500	-0.65125800	3.55982700
C	1.95171600	0.21348500	3.27053500
C	2.45002500	1.41093200	2.63850200
C	1.71293200	1.99967100	1.60353800
C	2.40186300	2.50103600	0.42870200
C	1.56211700	2.28520500	-0.71668700
C	2.13952500	1.90444300	-1.90695800
C	4.85163500	-1.59904700	-2.78935300
C	2.61573600	0.08529400	-3.33458700
C	6.00623700	-0.20322200	1.34648900
C	-2.15922000	3.02970000	-0.23148400
C	-2.82531300	2.00087100	0.46401800
C	-4.21073100	1.96346400	0.55207600
C	-5.02179200	2.97838000	-0.02206700
C	-4.33130800	4.04888500	-0.65743200

C	-2.95816900	4.06269500	-0.78366400
H	-2.25973500	1.23206900	0.97131800
H	-4.67489600	1.17505700	1.13533000
H	-4.93017400	4.85081500	-1.07825100
H	-2.47675200	4.88060600	-1.30841000
N	-0.75748400	3.08931900	-0.40168500
H	-1.42849500	1.07668600	-1.54071000
N	-6.38024900	3.07875300	0.05970200
C	-7.20479100	2.00663800	0.21523200
C	-6.92820000	0.65669900	-0.14760500
C	-8.51533600	2.27329600	0.70644400
C	-7.87369600	-0.34646700	-0.00620700
H	-5.96538700	0.40894600	-0.58073300
C	-9.45074400	1.27262300	0.86547400
H	-8.75291900	3.30098200	0.96333400
C	-9.15521300	-0.06355600	0.50967400
H	-7.61501000	-1.36293600	-0.28030100
H	-10.44101700	1.51173500	1.24859600
N	-10.13064400	-1.03468700	0.71858300
H	-10.84860600	-0.78333400	1.38411000
C	-10.26508600	-2.31095600	0.15482600
C	-10.96850200	-3.29051100	0.87833800
C	-9.77738400	-2.63376700	-1.12338800
C	-11.16960100	-4.55914500	0.34215700
H	-11.34789000	-3.05033200	1.86928800
C	-9.97034700	-3.91325500	-1.64180200
H	-9.27621300	-1.87826300	-1.71776800
C	-10.66349200	-4.88509100	-0.91821000
H	-11.71669400	-5.29990800	0.91942400
H	-9.58678200	-4.14352600	-2.63241500
H	-10.81225300	-5.87827400	-1.33142600
C	-0.16023400	4.39480600	-0.28578900
C	-0.16341200	5.07447300	0.93975000
C	0.40735100	5.02858300	-1.39830200
C	0.39845600	6.34046600	1.05738400
H	-0.61469500	4.60134700	1.80711900
C	0.97724400	6.29276700	-1.28730900
H	0.40035900	4.52126000	-2.35781500
C	0.98464200	6.97071000	-0.05545000
H	0.38364800	6.85177400	2.01723300
H	1.41015900	6.76866400	-2.16421000
N	1.50170200	8.26108200	0.04581500
H	2.19422400	8.50723300	-0.65002500
H	1.78584000	8.54324200	0.97538500

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction=	0.774048 (Hartree/Particle)
Thermal correction to Energy=	0.819478
Thermal correction to Enthalpy=	0.820422
Thermal correction to Gibbs Free Energy=	0.697097

Energy at B3LYP/6-311++G(d,p)
HF= -3433.069088

Name of compound	C60-L2-N4-H radical

Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	-0.38136400	-1.75311200	-1.25197100
C	0.29601900	-1.25379000	-2.43373100
C	1.31938100	-2.00674300	-3.02330500
C	1.71372900	-3.27771500	-2.43731800
C	1.06097100	-3.75777500	-1.30248100
C	-0.01521100	-2.98736100	-0.70138000
C	-0.70896900	-0.63213100	-0.41461500
C	-0.47922100	0.67828000	-1.17167100
C	0.38815900	0.17760600	-2.33039800
C	1.52758800	0.81213600	-2.76854400
C	2.50745100	-1.33740500	-3.49369000
C	3.15844000	-3.38690300	-2.54579800
C	3.89294400	-3.96972300	-1.51126200
C	3.21178400	-4.46996700	-0.32785500
C	1.82326600	-4.36804200	-0.22665100
C	1.21344900	-3.97352100	1.03340600
C	0.07690900	-3.12282600	0.73186000
C	-0.20407900	-2.01693500	1.54175200
C	-0.60748700	-0.76004400	0.95270200
C	0.12119700	1.89152900	-0.31547100
C	0.43736300	1.48906800	1.15550100
C	-0.00303400	0.32844900	1.75582500
C	0.75428500	-0.29092000	2.82083900
C	0.63423300	-1.73193700	2.69198400
C	1.71819900	-2.55645500	2.99209800
C	2.01882300	-3.69631500	2.14041600
C	3.46074600	-3.80495500	2.03495600
C	4.04674100	-4.18312600	0.82519000
C	3.64936000	-2.18392000	-3.19830700
C	6.30905500	-1.28343500	0.46501800
C	6.21210700	-1.15182000	-0.92200200
C	5.81310200	0.11432400	-1.50468200
C	5.52877700	1.20567200	-0.68034800
C	5.63078900	1.06963600	0.76396900
C	5.33093000	-0.65108400	2.50746700
C	5.20784600	-2.09228400	2.37816100
C	5.81327300	-2.48398200	1.11651900
C	5.24414500	-3.50695800	0.35622700
C	5.14808500	-3.37493400	-1.08784800
C	5.61919300	-2.21952400	-1.71489300
C	4.96895300	-0.16919800	-2.65446500
C	3.86555500	0.64101300	-2.92303600
C	3.56444000	1.77106600	-2.06419200
C	4.38725500	2.05293000	-0.96961700
C	3.78336400	2.43688400	0.28319100
C	4.55040800	1.83477400	1.36142200
C	3.89740400	1.35649800	2.49556900
C	4.29572100	0.08937100	3.08264000
C	4.05337300	-2.73718400	2.82764300
C	2.97752300	-1.96862100	3.42188400
C	3.09437400	-0.58269800	3.55058400
C	1.95973200	0.27154900	3.25122300
C	2.45009600	1.46219900	2.60067200

C	1.70754500	2.03193200	1.55903100
C	2.39098000	2.52025600	0.37530500
C	1.54988700	2.28331800	-0.76479000
C	2.12666800	1.88943800	-1.95125400
C	4.85597800	-1.61298200	-2.78799000
C	2.60984800	0.05114400	-3.35249000
C	6.01199700	-0.15103000	1.32440200
C	-2.18475700	2.98918300	-0.29870000
C	-2.83324900	2.01514000	0.47640300
C	-4.22380000	1.97564800	0.58375300
C	-5.02179800	2.91435800	-0.08082200
C	-4.37779000	3.90696700	-0.84060400
C	-2.99613500	3.94267500	-0.94834000
H	-2.26014300	1.28896400	1.03565700
H	-4.68182700	1.23045700	1.22493100
H	-4.97448200	4.64561700	-1.37133300
H	-2.52791700	4.71289300	-1.55193900
N	-0.77578000	3.07317300	-0.47139200
H	-1.43392800	1.04619500	-1.56614700
N	-6.42323700	2.94425000	0.02762900
H	-6.83951300	3.86375900	-0.02957700
C	-7.32119000	1.89965100	0.18275500
C	-6.99552500	0.54806200	-0.07146500
C	-8.64392400	2.20388400	0.58965700
C	-7.94633300	-0.44696400	0.05981500
H	-5.99244100	0.28743200	-0.38934100
C	-9.58488800	1.21113600	0.73982800
H	-8.90657900	3.23825200	0.80377300
C	-9.28854700	-0.15944800	0.46105400
H	-7.65619300	-1.47646800	-0.11849800
H	-10.59331700	1.44477300	1.06674200
N	-10.28131400	-1.05080300	0.67308700
C	-10.26117100	-2.33498300	0.17164100
C	-10.91884500	-3.33323700	0.93198100
C	-9.73217000	-2.70858900	-1.09035000
C	-10.98832300	-4.64592700	0.48424700
H	-11.35178700	-3.03982100	1.88350500
C	-9.83424600	-4.02071800	-1.54297200
H	-9.28961400	-1.94895400	-1.72681200
C	-10.44586600	-5.00117400	-0.75658100
H	-11.48023600	-5.39737700	1.09683700
H	-9.43791900	-4.28006400	-2.52179900
H	-10.51576900	-6.02505600	-1.11324700
C	-0.20912100	4.38469700	-0.28427500
C	-0.27571100	5.02864800	0.95898600
C	0.39441900	5.06143800	-1.35196800
C	0.25490300	6.30148900	1.13591000
H	-0.75329700	4.52343300	1.79369000
C	0.93578100	6.33171400	-1.18087500
H	0.44023200	4.58050700	-2.32397100
C	0.87614400	6.97416200	0.06805700
H	0.18966500	6.78476000	2.10822700
H	1.39838100	6.83976800	-2.02399000
N	1.36215800	8.27168100	0.22795700

H	2.08068100	8.54780700	-0.42943700
H	1.60560600	8.52786100	1.17656200

Frequency and Energy at B3LYP/6-31G(d)
Zero-point correction= 0.773866 (Hartree/Particle) Thermal correction to Energy= 0.819333 Thermal correction to Enthalpy= 0.820277 Thermal correction to Gibbs Free Energy= 0.696753
Energy at B3LYP/6-311++G(d,p)
HF= -3433.066735

Name of compound	C60-L2 cation

Cartesian Coordinates optimized at B3LYP/6-31G(d)			
C	-0.18721000	-1.65831600	-1.61497800
C	0.57889700	-1.01436200	-2.66558400
C	1.67334300	-1.67631000	-3.23611400
C	2.04835800	-2.99985800	-2.76466400
C	1.31013100	-3.61907500	-1.75697500
C	0.16539600	-2.93940600	-1.17352200
C	-0.61779000	-0.64888500	-0.68748100
C	-0.35713700	0.74654500	-1.26692800
C	0.62444800	0.39648800	-2.39354000
C	1.78195000	1.09495700	-2.64595600
C	2.88042000	-0.93797100	-3.51629900
C	3.49928900	-3.07224400	-2.75277000
C	4.15343600	-3.75695400	-1.72719800
C	3.38324600	-4.40184900	-0.67590300
C	1.98913700	-4.33693300	-0.69197800
C	1.25995200	-4.10028500	0.54324700
C	0.13328500	-3.23784200	0.23788700
C	-0.24953200	-2.23998800	1.13986000
C	-0.63081800	-0.93072800	0.66069600
C	0.14527100	1.84930700	-0.22017000
C	0.32908600	1.29986500	1.21975500
C	-0.12870700	0.06726900	1.63385600
C	0.54451700	-0.65774900	2.68859400
C	0.47392900	-2.07580500	2.38740000
C	1.54968300	-2.90985300	2.68771700
C	1.95549300	-3.93891100	1.74347700
C	3.40311300	-4.01103400	1.76004600
C	4.10401000	-4.23663000	0.57383200
C	4.01392400	-1.79426400	-3.21645900
C	6.31015200	-1.27792100	0.75444800
C	6.33374900	-0.98896000	-0.61157600
C	5.95347400	0.32851800	-1.08024600
C	5.56948900	1.31257500	-0.16680500
C	5.54634600	1.01349200	1.25572500
C	5.13723500	-0.90192200	2.75725400
C	5.06465800	-2.32009200	2.45378200
C	5.79056100	-2.55336500	1.21678400
C	5.31984600	-3.49095300	0.29645600
C	5.34949000	-3.19473300	-1.12569400
C	5.84345600	-1.96748900	-1.57162500
C	5.22344000	0.16607000	-2.32794200

C	4.12828500	0.98342200	-2.60388600
C	3.72151000	1.99953400	-1.65160600
C	4.43440200	2.16656400	-0.46112400
C	3.71212400	2.39552200	0.76640400
C	4.39688800	1.68647800	1.83509200
C	3.65881000	1.07014100	2.84295100
C	4.03633700	-0.24996700	3.31645500
C	3.89373600	-3.03251000	2.72013000
C	2.74919000	-2.35466500	3.29521100
C	2.81723900	-0.99163600	3.59181700
C	1.69158300	-0.12795800	3.28613300
C	2.20560300	1.13919300	2.82496100
C	1.54387400	1.81720500	1.79462200
C	2.31567000	2.44970600	0.74142100
C	1.58830700	2.32871800	-0.49213100
C	2.27763400	2.07559800	-1.65624400
C	5.16247600	-1.25420600	-2.63432500
C	2.93288400	0.42607800	-3.21110600
C	5.90785900	-0.25735900	1.70620000
C	-2.15128700	2.97474900	-0.09836400
C	-2.82668200	1.80774000	0.35096500
C	-4.20054700	1.76736700	0.48326200
C	-4.99328000	2.89309100	0.16950100
C	-4.33125200	4.07040000	-0.25564200
C	-2.96379000	4.11236000	-0.39007800
H	-2.26991400	0.93320200	0.64774600
H	-4.65927500	0.87411400	0.89016800
H	-4.91632900	4.95035300	-0.51234600
H	-2.49715400	5.02195500	-0.74445100
N	-0.78223100	3.05176100	-0.25914800
H	-1.28087600	1.14564300	-1.70461900
N	-6.36745900	2.92350500	0.30063800
H	-6.76520500	3.85484900	0.35800100
C	-7.29831900	1.89271500	0.37161900
C	-7.07473600	0.60359100	-0.15641900
C	-8.55321700	2.16929500	0.95960100
C	-8.05018500	-0.37393200	-0.07852800
H	-6.14247200	0.37486200	-0.65863000
C	-9.52752500	1.19818500	1.03617000
H	-8.74858200	3.15689200	1.37031900
C	-9.30336800	-0.10395600	0.52153300
H	-7.84499000	-1.35868700	-0.47932000
H	-10.48486200	1.43421100	1.49339400
N	-10.29852800	-1.04176800	0.64855000
H	-11.04605300	-0.79962800	1.28691400
C	-10.40929400	-2.32002100	0.05225200
C	-10.97864100	-3.35719200	0.80579800
C	-10.02900900	-2.55458600	-1.27765700
C	-11.15001100	-4.61774400	0.23965400
H	-11.27371400	-3.17412500	1.83604000
C	-10.19074700	-3.82491100	-1.82844600
H	-9.64532000	-1.74222400	-1.88579700
C	-10.74832400	-4.86046000	-1.07602100
H	-11.59139600	-5.41380700	0.83188500

H	-9.89799400	-3.99788700	-2.85998000
H	-10.87820900	-5.84527200	-1.51394200
C	-0.19230700	4.36709300	-0.28616500
C	-0.13180200	5.12800100	0.88943700
C	0.29803300	4.91629000	-1.47805200
C	0.42080100	6.40119400	0.88117800
H	-0.50857800	4.70806000	1.81753700
C	0.84548300	6.19159600	-1.49436300
H	0.24469200	4.34125700	-2.39713200
C	0.92216700	6.95912200	-0.31297600
H	0.46942400	6.97444600	1.80331000
H	1.21447200	6.60713600	-2.42836300
N	1.42376900	8.24356800	-0.33751100
H	2.01249900	8.50109600	-1.11774100
H	1.71546000	8.64862500	0.54142300

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction=	0.788366 (Hartree/Particle)
Thermal correction to Energy=	0.833953
Thermal correction to Enthalpy=	0.834898
Thermal correction to Gibbs Free Energy=	0.711251

Energy at B3LYP/6-311++G(d,p)

HF= -3433.493314

Name of compound	C60-L2 anion

Cartesian Coordinates optimized at B3LYP/6-31G(d)

C	0.30205400	-1.95155900	0.92267700
C	-0.24767200	-1.49865000	2.17995200
C	-1.26913800	-2.23557800	2.81157600
C	-1.78970400	-3.43864800	2.17362000
C	-1.25793200	-3.87519400	0.96028300
C	-0.18085500	-3.13321200	0.32264300
C	0.61710800	-0.80040900	0.12776200
C	0.52421400	0.47114000	0.97749500
C	-0.27293600	-0.06213500	2.17387000
C	-1.33550300	0.60306300	2.74352000
C	-2.37471500	-1.54028300	3.40852600
C	-3.22237100	-3.49165900	2.40375300
C	-4.07542900	-3.97865900	1.39658200
C	-3.52383600	-4.43100600	0.13815900
C	-2.13669700	-4.38550500	-0.07994600
C	-1.61410100	-3.93600100	-1.35284700
C	-0.40651600	-3.16179900	-1.09569400
C	-0.13264800	-2.02269800	-1.86727200
C	0.39531400	-0.82746500	-1.23414700
C	-0.08107500	1.76143800	0.24726700
C	-0.53215400	1.48213200	-1.21311200
C	-0.20690200	0.33496700	-1.91199900
C	-1.08714300	-0.18241900	-2.94507200
C	-1.02939800	-1.62682500	-2.92789900
C	-2.19359600	-2.38269400	-3.18783800
C	-2.48639000	-3.54586700	-2.37718600
C	-3.92314400	-3.59530300	-2.15359300
C	-4.42785900	-4.02518900	-0.92346200

C	-3.58696100	-2.30978900	3.15686600
C	-6.48640300	-1.03997800	-0.20172400
C	-6.26751200	-1.00849600	1.17914900
C	-5.74464000	0.19586800	1.80792700
C	-5.46922500	1.32208200	1.02080500
C	-5.70202900	1.29225000	-0.40734600
C	-5.65142900	-0.32600100	-2.27361800
C	-5.59196600	-1.77717100	-2.24371000
C	-6.11481100	-2.22211300	-0.96232100
C	-5.54508500	-3.32092000	-0.31641800
C	-5.32144900	-3.28943100	1.11982700
C	-5.67600700	-2.15099000	1.85064700
C	-4.84166100	-0.19944100	2.86705200
C	-3.66213500	0.54330500	3.09471800
C	-3.36921500	1.69652400	2.27523300
C	-4.25654700	2.09130200	1.26493500
C	-3.74070200	2.53462600	-0.00042600
C	-4.62483400	2.03015900	-1.04267900
C	-4.09192000	1.59489100	-2.25471200
C	-4.61344900	0.39534600	-2.89002400
C	-4.51562900	-2.45162500	-2.82571900
C	-3.44108100	-1.70346600	-3.46047500
C	-3.49725100	-0.30266900	-3.48896500
C	-2.29139500	0.47399200	-3.23102700
C	-2.65519300	1.64778100	-2.48492000
C	-1.79538000	2.11663300	-1.47083400
C	-2.35122100	2.55528000	-0.21046300
C	-1.44028000	2.19826300	0.83906000
C	-1.93646400	1.75471100	2.04614800
C	-4.79099500	-1.64624700	2.89051000
C	-2.41758200	-0.13781000	3.36731800
C	-6.20405800	0.12703800	-1.01701100
C	2.25276400	2.80672000	0.00447900
C	2.78234600	1.77043900	-0.78747000
C	4.13741000	1.72216600	-1.11437400
C	5.02993100	2.69764700	-0.65721700
C	4.51073500	3.73713100	0.12835200
C	3.16109900	3.79535000	0.44744200
H	2.13879400	1.00170200	-1.18895300
H	4.49168600	0.92707600	-1.76337100
H	5.18009500	4.50766200	0.50718900
H	2.80032700	4.61121900	1.06325500
N	0.89770100	2.89906500	0.38737100
H	1.52551800	0.76882300	1.31204600
N	6.39669400	2.70952100	-1.01926300
H	6.81612200	3.62773000	-1.06072400
C	7.30754600	1.65577400	-0.97593600
C	7.00026000	0.38042400	-0.46588300
C	8.61317300	1.87018500	-1.45896000
C	7.95409400	-0.63336500	-0.45765800
H	6.00754300	0.17926000	-0.08013100
C	9.57241800	0.86629700	-1.40921700
H	8.87651000	2.84419400	-1.86701200
C	9.26108600	-0.40835300	-0.91434000

H	7.67669100	-1.61780000	-0.09361900
H	10.58048100	1.07022000	-1.76465100
N	10.23402400	-1.43329500	-0.95369000
H	10.87853300	-1.38855600	-1.73017100
C	10.59666700	-2.31416900	0.06214000
C	11.53984600	-3.32183900	-0.22519000
C	10.07700300	-2.23966700	1.36816500
C	11.94498000	-4.22005200	0.75642600
H	11.94695100	-3.39546200	-1.23217600
C	10.48582500	-3.15284100	2.33857200
H	9.36718900	-1.46069000	1.62207400
C	11.41901700	-4.14982700	2.04911100
H	12.67459400	-4.98629400	0.50467000
H	10.06914900	-3.07368100	3.33992800
H	11.72892500	-4.85755200	2.81250700
C	0.36829300	4.23011400	0.50279500
C	0.22413300	5.04684300	-0.62643700
C	0.00026500	4.74933400	1.74969300
C	-0.28624600	6.33656000	-0.51776700
H	0.50637200	4.65554500	-1.59927300
C	-0.51775300	6.03653700	1.86505300
H	0.10975600	4.12624600	2.63142500
C	-0.67490100	6.84835500	0.73088600
H	-0.39785400	6.95190700	-1.40838300
H	-0.80545300	6.41800300	2.84263500
N	-1.15483800	8.16395100	0.84974000
H	-1.76470500	8.30101000	1.64795100
H	-1.60100500	8.50882400	0.00716600

Frequency and Energy at B3LYP/6-31G(d)

Zero-point correction=	0.782142 (Hartree/Particle)
Thermal correction to Energy=	0.828674
Thermal correction to Enthalpy=	0.829619
Thermal correction to Gibbs Free Energy=	0.702837

Energy at B3LYP/6-311++G(d,p)

HF= -3433.797526