

Role of Coupler to Design Organic Magnetic Molecules: LUMO Plays an Important Role in Magnetic Exchange

Suranjan Shil, Moumita Roy and Anirban Misra*

Department of Chemistry, University of North Bengal, Raja Rammohunpur, Darjeeling 734013,
West Bengal, India

Phone: +919434228745; Email: anirbanmisra@yahoo.com

Table S1 UB3LYP Level Absolute Energies in a.u., $\langle S^2 \rangle$ and Intramolecular Exchange-Coupling Constant (J cm⁻¹) Using 6-31+G(d) Basis Set, for the Diradicals (1–7)

Diradical		Triplet	BS	J (cm ⁻¹)	
A	1	E	-1606.00764	-1606.00742	47.33
		$\langle S^2 \rangle$	2.14	1.12	
	2	E	-1606.01601	-1606.01590	18.03
		$\langle S^2 \rangle$	2.13	1.12	
B	3	E	-1759.64745	-1759.64715	63.31
		$\langle S^2 \rangle$	2.17	1.13	
	4	E	-1759.66004	-1759.65996	17.38
		$\langle S^2 \rangle$	2.13	1.12	
	5	E	-1759.66331	-1759.6623	17.56
		$\langle S^2 \rangle$	2.12	1.12	
	6	E	-1759.66342	-1759.66336	13.16
		$\langle S^2 \rangle$	2.12	1.12	
	7	E	-1759.65373	-1759.65365	13.04
		$\langle S^2 \rangle$	2.12	1.12	

Table S2 UB3LYP Level Absolute Energies in a.u., $\langle S^2 \rangle$ and Intramolecular Exchange-Coupling Constant (J cm⁻¹) Using 6-311++G(d,p) Basis Set, for the Diradicals (1–7)

Diradical		Triplet	BS	$J(\text{cm}^{-1})$	
A	1	E	-1606.37789	-1606.37768	44.80
		$\langle S^2 \rangle$	2.14	1.12	
	2	E	-1606.38629	-1606.38619	23.26
		$\langle S^2 \rangle$	2.12	1.12	
B	3	E	-1760.04736	-1760.04709	57.43
		$\langle S^2 \rangle$	2.16	1.13	
	4	E	-1760.06016	-1760.06008	17.43
		$\langle S^2 \rangle$	2.13	1.12	
	5	E	-1760.06368	-1760.06359	18.06
		$\langle S^2 \rangle$	2.12	1.12	
	6	E	-1760.06361	-1760.06356	11.67
		$\langle S^2 \rangle$	2.12	1.12	
	7	E	-1760.05408	-1760.05401	13.39
		$\langle S^2 \rangle$	2.12	1.12	

Table S3 UBP86 Level Absolute Energies in a.u., $\langle S^2 \rangle$ and Intramolecular Exchange-Coupling Constant (J cm⁻¹) Using 6-311++G(d,p) Basis Set, for the Diradicals (1–7)

Diradical		Triplet	BS	$J(\text{cm}^{-1})$	
A	1	E	-1606.40114	-1606.40111	7.68
		$\langle S^2 \rangle$	2.03	1.03	
	2	E	-1606.40874	-1606.40873	3.73
		$\langle S^2 \rangle$	2.03	1.03	
B	3	E	-1760.07013	-1760.07009	8.93
		$\langle S^2 \rangle$	2.04	1.03	
	4	E	-1760.08143	-1760.08142	2.79
		$\langle S^2 \rangle$	2.03	1.03	
	5	E	-1760.08427	-1760.08426	2.92
		$\langle S^2 \rangle$	2.03	1.03	
	6	E	-1760.08453	-1760.08452	1.80
		$\langle S^2 \rangle$	2.03	1.03	
	7	E	-1760.07603	-1760.07602	2.12

	$\langle S^2 \rangle$	2.03	1.03	
--	-----------------------	------	------	--

Table S4 The Energy of SOMOs and LUMO in a.u. and Their Differences in eV at UB3LYP Level Using a 6-31+G(d) Basis set for the Diradicals

Diradical		E_{SOMO1}	E_{SOMO2} (E_{HOMO})	E_{LUMO}	$\Delta E_{\text{SS}}(\text{eV})$	$\Delta E_{\text{HL}}(\text{eV})$
A	1	-0.19681	-0.19679	-0.08409	0.0	3.07
	2	-0.19724	-0.19642	-0.07040	0.02	3.43
B	3	-0.19724	-0.19053	-0.09462	0.18	2.61
	4	-0.19753	-0.19667	-0.08075	0.02	3.15
	5	-0.19758	-0.19631	-0.07155	0.02	3.41
	6	-0.19815	-0.19689	-0.07240	0.03	3.39
	7	-0.19667	-0.19667	-0.07552	0.0	3.30

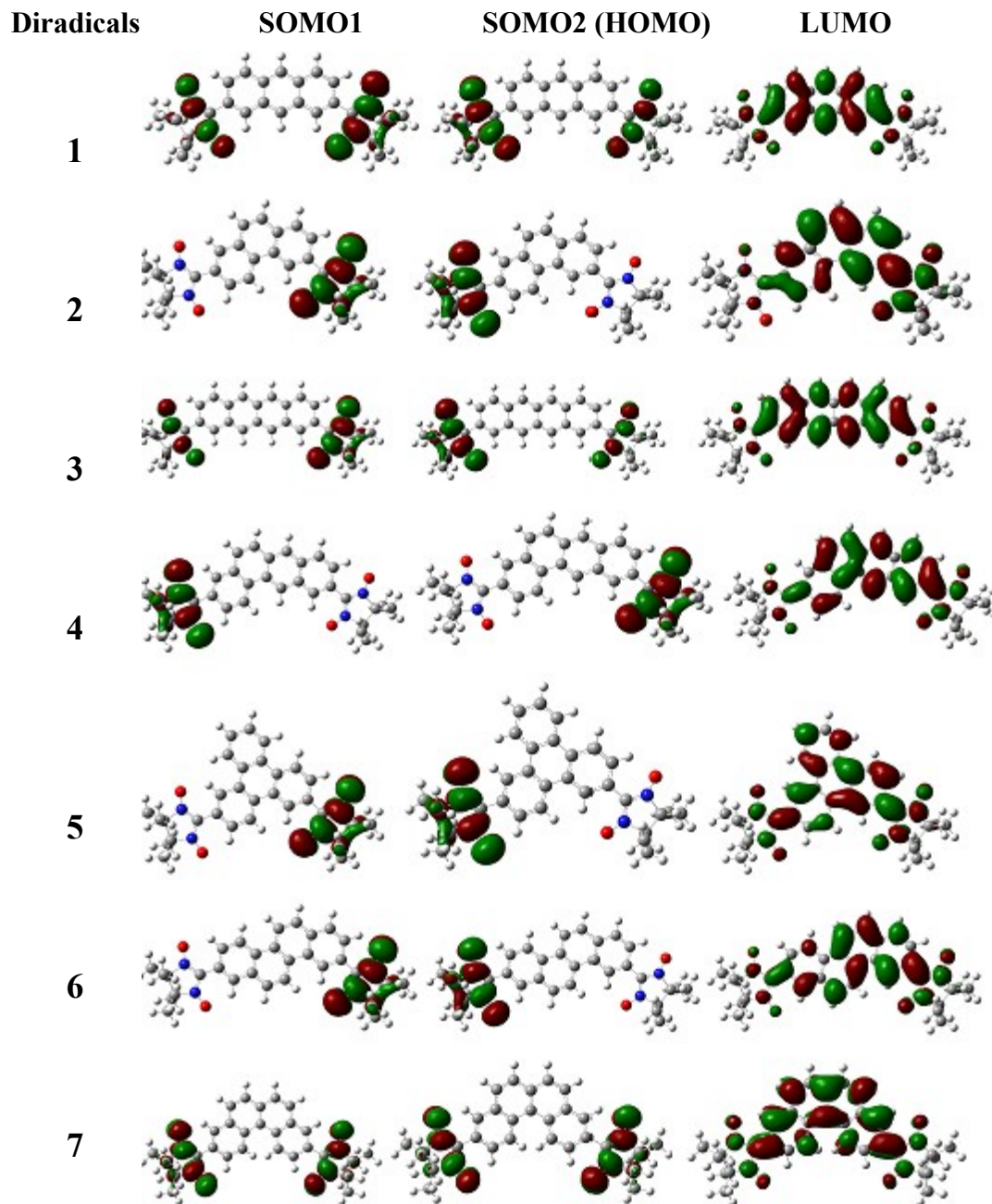


Fig. S1 Spatial distribution of molecular orbitals (the green and violet colour represents the different phase of the orbital coefficients), the iso value is 0.02 (BP86/6-311++G(d,p)).

Optimized Coordinate of the Polyacene Couplers (B3LYP/6-31+G(d,p))

Polyacene I

C	0.00000000	3.66447000	0.71368900
C	0.00000000	2.48163400	1.40815300
C	0.00000000	1.22476200	0.72285600
C	0.00000000	1.22476200	-0.72285600
C	0.00000000	2.48163400	-1.40815300
C	0.00000000	3.66447000	-0.71368900
C	0.00000000	0.00000000	1.40478300
C	0.00000000	0.00000000	-1.40478300
C	0.00000000	-1.22476200	-0.72285600
C	0.00000000	-1.22476200	0.72285600
C	0.00000000	-2.48163400	1.40815300
H	0.00000000	-2.48052600	2.49519500
C	0.00000000	-3.66447000	0.71368900
C	0.00000000	-3.66447000	-0.71368900
C	0.00000000	-2.48163400	-1.40815300
H	0.00000000	0.00000000	2.49266600
H	0.00000000	4.61014400	1.24796500
H	0.00000000	2.48052600	2.49519500
H	0.00000000	2.48052600	-2.49519500
H	0.00000000	4.61014400	-1.24796500
H	0.00000000	0.00000000	-2.49266600
H	0.00000000	-4.61014400	1.24796500
H	0.00000000	-4.61014400	-1.24796500
H	0.00000000	-2.48052600	-2.49519500

Polyacene II

C	0.00000000	3.56481300	-0.29758600
C	0.00000000	2.84003700	0.87943900
C	0.00000000	1.42416200	0.86727800
C	0.00000000	0.72936100	-0.38010100
C	0.00000000	1.50040200	-1.56771300
C	0.00000000	2.88467300	-1.53144100
H	0.00000000	1.23151200	3.03306200

H	0.00000000	4.65052900	-0.27301500
H	0.00000000	3.35212400	1.83842300
C	0.00000000	0.68067400	2.09603800
C	0.00000000	-0.72936100	-0.38010100
H	0.00000000	1.00748000	-2.53334400
H	0.00000000	3.44714300	-2.46061000
C	0.00000000	-1.42416200	0.86727800
C	0.00000000	-0.68067400	2.09603800
H	0.00000000	-1.23151200	3.03306200
C	0.00000000	-2.84003700	0.87943900
C	0.00000000	-3.56481300	-0.29758600
H	0.00000000	-4.65052900	-0.27301500
C	0.00000000	-2.88467300	-1.53144100
H	0.00000000	-3.44714300	-2.46061000
C	0.00000000	-1.50040200	-1.56771300
H	0.00000000	-1.00748000	-2.53334400
H	0.00000000	-3.35212400	1.83842300

Polyacene III

C	1.23646200	-1.40762700	0.00000000
C	0.00000600	-0.72662400	0.00000000
C	0.00000000	0.72661500	0.00000000
C	1.23643800	1.40763700	0.00000000
C	2.45277500	0.72641900	0.00000000
C	-1.23646600	-1.40764700	0.00000000
C	-1.23648000	1.40762800	0.00000000
C	-2.45276700	0.72637600	0.00000000
C	-2.45275800	-0.72640600	0.00000000
C	-3.71473100	-1.41060100	0.00000000
H	-3.71344700	-2.49765900	0.00000000
C	-4.89428000	-0.71610700	0.00000000
C	-4.89428900	0.71604600	0.00000000
C	-3.71474700	1.41055400	0.00000000
H	-1.23652400	-2.49549400	0.00000000
H	1.23653800	-2.49547700	0.00000000
H	1.23652200	2.49548500	0.00000000
H	-1.23655700	2.49547500	0.00000000
H	-5.84110000	-1.24831000	0.00000000
H	-5.84111400	1.24823900	0.00000000
H	-3.71348100	2.49761200	0.00000000
C	3.71470700	1.41058100	0.00000000
C	4.89430100	0.71609400	0.00000000
H	5.84107700	1.24837200	0.00000000

C	4.89431200	-0.71601600	0.00000000
H	5.84109900	-1.24827400	0.00000000
C	3.71473700	-1.41052700	0.00000000
H	3.71353400	-2.49758900	0.00000000
H	3.71348100	2.49764100	0.00000000
C	2.45277600	-0.72639800	0.00000000

Polyacene IV

C	-0.84735800	-4.68715300	0.00000000
C	0.29838100	-3.92796100	0.00000000
C	0.23041300	-2.50190100	0.00000000
C	-1.06089400	-1.86754000	0.00000000
C	-2.22828400	-2.68952300	0.00000000
C	-2.12607800	-4.06032700	0.00000000
C	1.37595900	-1.68656000	0.00000000
C	-1.13559100	-0.46034500	0.00000000
C	0.00000000	0.34914900	0.00000000
C	1.29273300	-0.29370700	0.00000000
C	2.48603400	0.51524600	0.00000000
H	3.44826600	0.01005300	0.00000000
C	2.41945000	1.87116000	0.00000000
C	-0.06168100	1.81450100	0.00000000
H	2.35763800	-2.15519200	0.00000000
H	-0.78286900	-5.77131100	0.00000000
H	1.27556600	-4.40408600	0.00000000
H	-3.20418200	-2.21065100	0.00000000
H	-3.02249100	-4.67349300	0.00000000
H	-2.12490000	-0.01466900	0.00000000
H	3.32841300	2.46704600	0.00000000
C	-1.27901400	2.53127800	0.00000000
C	-1.30415000	3.91854800	0.00000000
H	-2.25744800	4.43890600	0.00000000
C	-0.10328600	4.64976200	0.00000000
H	-0.12398800	5.73549400	0.00000000
C	1.10537500	3.97333400	0.00000000
H	2.04142200	4.52608000	0.00000000
H	-2.22263900	1.99741200	0.00000000
C	1.15252600	2.56110600	0.00000000

Polyacene V

C	3.52776100	-0.00000100	0.00036500
C	2.83586500	-1.21185400	0.00030500

C	1.43042600	-1.23713900	0.00015900
C	0.71401700	0.00000000	0.00007300
C	1.43042700	1.23713900	0.00013500
C	2.83586500	1.21185400	0.00028100
C	0.68160300	-2.46595700	0.00009200
C	-0.71401700	0.00000000	-0.00007400
C	-1.43042600	-1.23713900	-0.00013600
C	-0.68160400	-2.46595700	-0.00004800
C	-2.83586500	-1.21185400	-0.00028100
H	-3.38274200	-2.15118500	-0.00032800
C	-3.52776100	0.00000000	-0.00036300
C	-2.83586400	1.21185400	-0.00030300
C	-1.43042700	1.23714000	-0.00015900
C	-0.68160200	2.46595800	-0.00009400
C	0.68160300	2.46595800	0.00004600
H	1.23024600	3.40435600	0.00009200
H	-1.23024500	3.40435600	-0.00015900
H	1.23024400	-3.40435600	0.00015800
H	4.61395300	0.00000000	0.00047800
H	3.38274200	-2.15118500	0.00037200
H	3.38274400	2.15118400	0.00032900
H	-1.23024600	-3.40435500	-0.00009600
H	-4.61395300	0.00000100	-0.00047400
H	-3.38274300	2.15118500	-0.00036800

Polyacene VI

C	-3.76460900	2.77788500	0.00000000
C	-3.72358500	1.39812500	0.00000000
C	-2.48738800	0.70384900	0.00000000
C	-1.26003500	1.43509100	0.00000000
C	-1.33941600	2.85245100	0.00000000
C	-2.55718400	3.50818500	0.00000000
C	-2.44419400	-0.72361300	0.00000000
C	0.00000000	0.70936800	0.00000000
C	-0.00001500	-0.70944700	0.00000000
C	-1.25635400	-1.39711600	0.00000000
C	1.25996500	-1.43511100	0.00000000
C	2.48734000	-0.70380700	0.00000000
C	2.44410500	0.72357400	0.00000000
C	1.25619000	1.39706700	0.00000000
H	-3.38232500	-1.27262900	0.00000000
H	-4.71706500	3.29964900	0.00000000
H	-4.64417100	0.81984700	0.00000000
H	-2.58213700	4.59409300	0.00000000

H	-1.27502300	-2.48012900	0.00000000
H	3.38217100	1.27270200	0.00000000
C	3.72360900	-1.39806900	0.00000000
C	3.76472200	-2.77776700	0.00000000
H	4.71718100	-3.29952600	0.00000000
C	2.55729400	-3.50816000	0.00000000
H	2.58237500	-4.59406500	0.00000000
C	1.33952700	-2.85254000	0.00000000
H	0.43464000	-3.44864000	0.00000000
H	1.27487000	2.48009300	0.00000000
H	4.64412800	-0.81968100	0.00000000
H	-0.43447500	3.44848600	0.00000000

Polyacene VII

C	-3.99054600	-1.44742100	-0.00001500
C	-3.80770600	-0.08214300	0.00003100
C	-2.51355100	0.49900700	0.00002800
C	-1.32401100	-0.31796100	-0.00001000
C	-1.57668600	-1.72135500	-0.00007400
C	-2.84928100	-2.26744600	-0.00007400
H	-3.34201200	2.50420400	0.00007700
H	-4.98686800	-1.87848600	-0.00001500
H	-4.66417200	0.58692300	0.00006600
C	-2.42518900	1.92149300	0.00005200
C	0.00000000	0.33625700	0.00000000
H	-0.77621100	-2.43347400	-0.00013700
H	-2.95533700	-3.34840200	-0.00012500
C	0.00000000	1.76393700	0.00000000
C	-1.21017400	2.52575700	0.00002900
H	-1.13057500	3.60907000	0.00003500
C	1.21017400	2.52575700	-0.00002800
C	2.42518900	1.92149300	-0.00005200
C	2.51355100	0.49900700	-0.00002800
C	1.32401100	-0.31796100	0.00001000
C	1.57668600	-1.72135500	0.00007300
C	2.84928100	-2.26744600	0.00007400
C	3.99054600	-1.44742100	0.00001500
C	3.80770600	-0.08214300	-0.00003100
H	2.95533700	-3.34840200	0.00012500
H	0.77621100	-2.43347400	0.00013700
H	4.66417200	0.58692300	-0.00006500
H	4.98686800	-1.87848600	0.00001500
H	1.13057500	3.60907000	-0.00003500
H	3.34201200	2.50420400	-0.00007700

Optimized Coordinate of the Diradicals

B3LYP/6-31+G(d,p)

Diradical 1

C	-3.66685400	2.22150100	0.00447900
C	-1.22436700	0.80133800	0.00154500
C	-1.22233600	2.24477800	-0.00068400
C	-2.48599100	2.91275000	-0.00373500
C	-3.67753900	0.77865600	0.01046100
C	-2.46591500	0.10115300	0.00327800
H	-4.60927300	2.75131300	0.01853000
H	-2.50038200	4.00038700	-0.00903600
C	-4.94276400	0.04676700	0.00872000
H	-2.45334500	-0.98078800	-0.01381500
N	-5.09256400	-1.29157400	-0.20761400
N	-6.18304800	0.58040000	0.21693900
C	-7.27926600	-0.40784700	-0.09386700
C	-6.50306800	-1.75362400	0.05848400
O	-4.17403800	-2.14492400	-0.46372500
O	-6.47176700	1.79178000	0.50926300
C	-7.73742300	-0.10677300	-1.53416600
C	-8.44641000	-0.21252900	0.87410900
C	-6.51084700	-2.32277800	1.49039200
C	-6.88795000	-2.84751700	-0.93781000
H	-6.92444900	-0.23137000	-2.25643600
H	-8.56374600	-0.76421700	-1.82297800
H	-8.08544000	0.92932000	-1.58328400
H	-8.89528400	0.77082800	0.71540900
H	-9.20951000	-0.97685400	0.68891800
H	-8.13491700	-0.27340600	1.91914200
H	-6.23099900	-1.56867300	2.23288600
H	-7.50143800	-2.71215800	1.74616700
H	-5.79011200	-3.14390600	1.54713900
H	-6.26212000	-3.72834600	-0.77643300
H	-7.93503400	-3.13232800	-0.78537100
H	-6.75800900	-2.52962800	-1.97456400
C	-0.00000600	2.92957900	-0.00011800
C	1.22232500	2.24477900	0.00048300

C	1.22435900	0.80133900	-0.00168300
C	-0.00000400	0.11549300	-0.00005700
C	2.46590600	0.10115300	-0.00337300
C	3.66684400	2.22150100	-0.00464100
C	2.48598000	2.91274900	0.00351600
H	2.45333800	-0.98078700	0.01375100
H	2.50037200	4.00038600	0.00876400
H	-0.00000600	4.01812700	-0.00014200
H	-0.00000300	-0.97249600	-0.00003500
C	3.67753500	0.77865400	-0.01055500
C	4.94276100	0.04676600	-0.00874300
N	6.18308100	0.58043000	-0.21668600
N	5.09253500	-1.29160900	0.20740800
C	6.50308400	-1.75361600	-0.05853100
C	7.27925100	-0.40786000	0.09414300
O	6.47185700	1.79185600	-0.50876500
O	4.17397600	-2.14500900	0.46323600
C	8.44654800	-0.21239100	-0.87362000
C	7.73718500	-0.10700100	1.53456000
C	6.51110400	-2.32255300	-1.49052300
C	6.88781000	-2.84765500	0.93766100
H	8.13522100	-0.27311400	-1.91871100
H	8.89538900	0.77094600	-0.71470400
H	9.20962400	-0.97673800	-0.68842200
H	8.56346800	-0.76448400	1.82339700
H	8.08518500	0.92908700	1.58388800
H	6.92410000	-0.23171500	2.25668600
H	6.23133900	-1.56834700	-2.23294400
H	7.50175200	-2.71185000	-1.74620400
H	5.79041300	-3.14370400	-1.54750700
H	6.26198400	-3.72844800	0.77607500
H	7.93490900	-3.13246700	0.78532400
H	6.75773500	-2.52991100	1.97444300
H	4.60926200	2.75131300	-0.01868700

Diradical 2

C	3.70858700	2.45195300	-0.04179600
---	------------	------------	-------------

C	2.64934000	3.33389500	-0.05939100
C	1.30633000	2.88981000	-0.05214400
C	1.04648800	1.48751600	-0.03478100
C	2.13858200	0.59566600	-0.02092800
C	3.46419500	1.04832600	-0.02049800
H	0.43899800	4.88388700	-0.07287500
H	4.72618000	2.81632600	-0.03222800
H	2.84568500	4.40371700	-0.07433700
C	0.21408900	3.81986300	-0.05961500
C	-0.33511900	1.02287800	-0.03239400
H	1.96739700	-0.46952900	-0.01965600
C	-1.39003200	1.98148500	-0.03360300
C	-1.07697900	3.38509000	-0.04830000
H	-1.89991600	4.09592900	-0.05222900
C	-2.73680500	1.56127400	-0.02444900
C	-3.07734100	0.20413000	-0.01623700
C	-2.01934800	-0.75044800	-0.02193000
H	-2.25729800	-1.80463500	-0.01404900
C	-0.69963300	-0.34374800	-0.02969600
H	0.06640200	-1.11182800	-0.03495600
H	-3.51808900	2.30949800	-0.03047000
C	-6.41634900	-1.59609300	-0.18673200
C	-6.84810100	-0.15582400	0.22700900
C	6.78432000	-0.79076000	-0.10434900
C	5.77980700	-1.95433100	0.16204500
C	-4.47695900	-0.22232100	-0.00366500
C	4.57355200	0.09436800	-0.00078000
N	5.89632600	0.40291900	0.14422900
N	4.47144500	-1.26086400	-0.12267400
N	-5.56658500	0.59907800	-0.02269900
N	-4.92637000	-1.51203600	0.03221500
O	-4.22744600	-2.58182800	0.08769100
O	-5.57834900	1.87746100	-0.08121200
O	6.41220200	1.55941600	0.32510300
O	3.40802100	-1.95064800	-0.30304500
C	-6.61826500	-1.90407900	-1.68306600
H	-6.11253700	-2.84451500	-1.92100200
H	-7.68267400	-2.01328100	-1.91452300
H	-6.20164900	-1.11859000	-2.32148900
C	-7.98060200	0.45218100	-0.60105800
H	-8.89208600	-0.14162600	-0.46932800
H	-8.17862400	1.47116800	-0.26043900
H	-7.74084300	0.49541100	-1.66575900
C	-7.00398400	-2.72509700	0.66033700
H	-8.09406100	-2.73840600	0.54986000
H	-6.60919100	-3.68458300	0.31815800

H	-6.75987600	-2.62092300	1.71979600
C	-7.15562700	0.00084300	1.72898700
H	-7.24206100	1.06654800	1.96067900
H	-8.10170300	-0.48745500	1.98405600
H	-6.36457400	-0.42375200	2.35520100
C	5.93215400	-3.17306300	-0.74892200
H	6.91598200	-3.62920300	-0.59138100
H	5.16497800	-3.91201500	-0.50614300
H	5.82889200	-2.91808100	-1.80595000
C	7.24936900	-0.68625600	-1.56963000
H	7.78030100	0.26087900	-1.70375000
H	7.93232800	-1.50493500	-1.81804700
H	6.40747200	-0.71036500	-2.26869500
C	7.99377800	-0.74414200	0.82965100
H	8.59966900	-1.64647800	0.69086000
H	8.60895800	0.12655400	0.59096800
H	7.70544900	-0.67298200	1.88060800
C	5.71816100	-2.40548200	1.63441800
H	4.85563100	-3.06569400	1.76423700
H	6.62248800	-2.95823100	1.90844100
H	5.60758900	-1.55749400	2.31774500

Diradical 3

C	1.23458600	0.02212300	-0.00296600
C	-0.00000400	-0.66089500	-0.00006800
C	-0.00000200	-2.11482400	-0.00007400
C	1.23712800	-2.79551600	0.00064600
C	2.45035300	-2.11139500	-0.00102800
C	-1.23459600	0.02211900	0.00283900
C	-1.23713000	-2.79552000	-0.00079600
C	-2.45035700	-2.11140400	0.00089400
C	-2.45211400	-0.66231500	0.00553700
C	-3.69704100	0.03756300	0.00950100
H	-3.68417700	1.11950400	-0.00554100
C	-4.90707800	-0.63867100	0.01575800
C	-4.89701400	-2.08607800	0.00629500
C	-3.71954600	-2.77743700	-0.00330400
H	-1.23627200	1.11029200	0.00311600
H	1.23625900	1.11029600	-0.00323500
H	1.23880500	-3.88400500	0.00300500
H	-1.23880300	-3.88400900	-0.00316700
H	-5.84039200	-2.61407700	0.01836800
H	-3.73485100	-3.86507400	-0.01121800
C	3.71954300	-2.77742400	0.00317700

C	4.89701000	-2.08606200	-0.00638900
H	5.84038800	-2.61405900	-0.01844400
C	4.90707300	-0.63865400	-0.01582700
C	3.69703100	0.03757600	-0.00960100
H	3.68416500	1.11951700	0.00543300
H	3.73485300	-3.86506100	0.01107500
C	2.45210600	-0.66230800	-0.00565900
C	-8.50757800	0.54801800	-0.10209800
C	-7.73299500	1.89263000	0.06649400
C	8.50756200	0.54801600	0.10236000
C	7.73302700	1.89262000	-0.06652500
C	-6.17128400	0.09276700	0.01367900
C	6.17127700	0.09278700	-0.01370000
N	7.41380600	-0.44212100	-0.21025100
N	6.32059700	1.43311500	0.19291900
N	-7.41378000	-0.44210200	0.21047100
N	-6.32061900	1.43307500	-0.19310600
O	-5.40056900	2.28912600	-0.43509200
O	-7.70493400	-1.65466200	0.49495000
O	7.70498700	-1.65471800	-0.49454300
O	5.40052200	2.28922100	0.43462400
C	-7.75191500	2.45019000	1.50283200
H	-7.03311900	3.27211800	1.57144800
H	-8.74504800	2.83565600	1.75464600
H	-7.47607000	1.69049300	2.24111000
C	-9.68264400	0.34540300	0.85478700
H	-10.44409500	1.11131000	0.66932000
H	-10.13038000	-0.63658800	0.68486500
H	-9.37969500	0.39804400	1.90278500
C	-8.11129000	2.99422200	-0.92381300
H	-9.15933000	3.27798500	-0.77605300
H	-7.48650200	3.87374100	-0.75157400
H	-7.97461700	2.68440100	-1.96214200
C	-8.95397900	0.25754800	-1.54831300
H	-9.30118800	-0.77827800	-1.60795700
H	-9.77824400	0.91682500	-1.83881300
H	-8.13528400	0.38782000	-2.26307700
C	8.11116900	2.99433300	0.92370300
H	9.15921700	3.27811300	0.77603300
H	7.48637100	3.87380900	0.75128700
H	7.97438400	2.68462800	1.96205100
C	8.95373000	0.25772700	1.54868500
H	9.30089100	-0.77810400	1.60852500
H	9.77797400	0.91701500	1.83921700
H	8.13492900	0.38812700	2.26330400
C	9.68278800	0.34524600	-0.85430300

H	10.44423100	1.11115300	-0.66880600
H	10.13046300	-0.63673700	-0.68417900
H	9.38001900	0.39775900	-1.90236000
C	7.75216600	2.45000200	-1.50292700
H	7.03341900	3.27195500	-1.57174800
H	8.74535300	2.83538600	-1.75465300
H	7.47638700	1.69022400	-2.24114600

Diradical 4

C	4.84763400	2.18231500	-0.05475100
C	3.77570400	3.03554900	-0.08691200
C	2.43443400	2.55055400	-0.07651500
C	2.22782000	1.12970000	-0.04421600
C	3.35173100	0.25910500	-0.02137700
C	4.64998400	0.75721700	-0.01846900
C	1.31125200	3.39331900	-0.09440300
C	0.91034100	0.62503000	-0.03654600
C	-0.20635500	1.45985200	-0.05329900
C	0.00987000	2.88791300	-0.08099700
C	-1.12602400	3.77502200	-0.09236200
H	-0.94012900	4.84642600	-0.11327700
C	-2.39643300	3.29601200	-0.07516700
C	-1.57995600	0.95434500	-0.04224500
H	1.45840900	4.47165600	-0.11681300
H	5.85613600	2.57204000	-0.04289600
H	3.94363900	4.10988800	-0.11519900
H	3.18609000	-0.81050300	-0.01863300
H	0.78996200	-0.45348700	-0.01471400
H	-3.24435500	3.97672900	-0.08186700
C	-1.90178400	-0.42002700	-0.02530600
C	-3.20891900	-0.87184900	-0.01164000
H	-3.41205700	-1.93316200	0.00519000
C	-4.29412400	0.04723300	-0.01272000
C	-3.99371000	1.41626000	-0.03280900
H	-4.79838200	2.13919600	-0.04105600
H	-1.11232500	-1.16421700	-0.02276900
C	-2.66353500	1.87734500	-0.04909600
C	-7.57864000	-1.85049000	-0.17877200
C	-8.04902600	-0.43130800	0.26464200
C	8.04589500	-0.93275600	-0.02280600
C	7.08106200	-2.15309500	0.10216500
C	-5.67977400	-0.42149300	0.00697500
C	5.79712400	-0.14859200	0.00932100
C	-7.78898900	-2.13936600	-1.67775900

H	-7.25764400	-3.05961200	-1.93777000
H	-8.85225300	-2.27731500	-1.89877700
H	-7.40440800	-1.33066700	-2.30728000
C	-9.20886700	0.15605100	-0.54030900
H	-10.10069400	-0.46684100	-0.40836300
H	-9.43307800	1.16283200	-0.18020800
H	-8.98298500	0.22408900	-1.60673100
C	-8.12144100	-3.01096000	0.65570200
H	-9.21174700	-3.05653000	0.55682200
H	-7.70103000	-3.95192100	0.29321000
H	-7.86881000	-2.91665900	1.71411900
C	-8.34439300	-0.30984100	1.77232300
H	-8.46202300	0.74841800	2.02351500
H	-9.27155600	-0.83238500	2.02889000
H	-7.53335400	-0.71962600	2.38262600
C	8.58721600	-0.70469200	-1.44764300
H	9.07755000	0.27261400	-1.48537800
H	9.32286300	-1.47177400	-1.71003600
H	7.78868400	-0.71737100	-2.19621900
C	7.33735500	-3.29392300	-0.88285700
H	8.32543100	-3.72844200	-0.69418400
H	6.58409800	-4.07331600	-0.74564800
H	7.29196000	-2.96415800	-1.92302900
C	9.19843100	-0.90221200	0.98162700
H	9.84949100	-1.76881100	0.82110500
H	9.78803400	0.00590500	0.83624200
H	8.84938700	-0.91225700	2.01651200
C	6.95937500	-2.71376100	1.53241000
H	6.12423000	-3.41976300	1.56333100
H	7.87283800	-3.24429200	1.81981000
H	6.76957300	-1.92441300	2.26667300
O	7.54235600	1.36214300	0.55745600
O	4.73635900	-2.20674200	-0.49463300
O	-5.35654000	-2.77291800	0.04740800
O	-6.84485100	1.64497400	-0.01835500
N	-6.08922200	-1.72458000	0.02418500
N	-6.79404800	0.36677700	0.01463100
N	5.75998000	-1.49438400	-0.20770800
N	7.09333600	0.20323300	0.25470000

Diradical 5

C	2.21303700	0.21179000	-0.01393000
---	------------	------------	-------------

C	3.54116200	0.65541700	-0.00411700
C	3.77683100	2.05404400	-0.00868000
H	4.79060300	2.42856300	0.00850000
C	2.71188400	2.93299800	-0.02145400
C	1.36577700	2.50163400	-0.02633700
C	1.12120500	1.10224100	-0.02352300
H	2.94219800	3.99175800	-0.02295100
C	0.24566500	3.44618500	-0.03199500
C	-1.09120500	2.96069900	-0.02607500
C	-1.34447300	1.51262700	-0.02088100
C	-0.25634700	0.60081600	-0.02981100
C	0.45893300	4.84476400	-0.04256100
C	-0.59484000	5.74318800	-0.04623000
H	-0.39706100	6.81187100	-0.05477500
C	-1.91320800	5.26384500	-0.03954900
H	-2.75058800	5.95672800	-0.04293200
C	-2.14945200	3.89861300	-0.02984900
H	-3.17790700	3.55748600	-0.02716400
H	1.46851300	5.23839500	-0.04850600
C	-2.66035900	1.01010800	-0.01204600
C	-2.93885400	-0.36295300	-0.01783600
C	-1.84445200	-1.26522500	-0.03807500
H	-2.02471800	-2.33065500	-0.04331200
C	-0.55107500	-0.78159100	-0.04301900
H	-3.49871800	1.68678400	-0.00557600
H	0.25195100	-1.50904400	-0.05862800
H	2.04327900	-0.85231000	-0.02214300
C	6.85731300	-1.18701600	-0.11546900
C	5.85448000	-2.34934400	0.16476100
C	-6.20085700	-2.29724700	-0.20582500
C	-6.68988800	-0.88735300	0.24669500
C	4.64854100	-0.30023200	0.00833600
C	-4.32031500	-0.84531600	-0.00456200
N	-4.71400000	-2.15390500	0.00233500
N	-5.44443300	-0.07175900	0.00623000
N	4.54317300	-1.65558400	-0.10584700
N	5.97259000	0.00839600	0.13637900
C	-6.40368500	-2.57775000	-1.70747300
H	-5.85997600	-3.48922800	-1.97283100
H	-7.46453500	-2.72758100	-1.93233200
H	-6.02776200	-1.75968400	-2.33008400
C	-7.85493700	-0.30890100	-0.55723400
H	-8.73866000	-0.94487100	-0.43330600
H	-8.09394200	0.69175700	-0.18973400
H	-7.62646700	-0.22919400	-1.62229400
C	-6.73118800	-3.47057900	0.61867400

H	-7.82051900	-3.52968600	0.51612000
H	-6.29742200	-4.40335100	0.25077700
H	-6.48288300	-3.38075800	1.67851400
C	-6.99113100	-0.78129100	1.75435800
H	-7.12353000	0.27328500	2.01351400
H	-7.91198700	-1.31816900	2.00394100
H	-6.17646900	-1.18515800	2.36377100
C	7.30940500	-1.08802000	-1.58519400
H	7.84012400	-0.14192000	-1.72714700
H	7.98923700	-1.90829700	-1.83683400
H	6.46136600	-1.11343100	-2.27676000
C	5.99501400	-3.56969300	-0.74596700
H	6.97902500	-4.02833000	-0.59714000
H	5.22810400	-4.30611600	-0.49481800
H	5.88250600	-3.31571700	-1.80228400
C	8.07524600	-1.13746700	0.80738400
H	8.67984700	-2.04027200	0.66614200
H	8.68825400	-0.26760200	0.56012900
H	7.79644700	-1.06277400	1.86065700
C	5.80958000	-2.79820900	1.63841900
H	4.94898300	-3.45874900	1.77890600
H	6.71731000	-3.34993200	1.90300100
H	5.70600400	-1.94934600	2.32174600
O	-3.96815400	-3.19252000	0.02155900
O	-5.51427500	1.20694900	-0.01733900
O	6.49001000	1.16654900	0.30116100
O	3.47632200	-2.34462500	-0.26831300

Diradical 6

C	4.81351300	2.34704300	-0.00479600
C	3.75144900	3.22198600	-0.01351200
C	2.40919500	2.76950700	-0.01653300
C	2.15043300	1.36680400	-0.01504700
C	3.25171400	0.48112900	-0.00723500
C	4.57376400	0.93984100	-0.00024100
C	1.31316400	3.68152100	-0.02026100
C	0.77399600	0.89450600	-0.02146800
C	-0.29011700	1.83362600	-0.02057500
C	0.02264300	3.23159000	-0.02074700
C	-1.66405100	1.36692900	-0.01998100
C	-1.92796600	-0.03458300	-0.02687500
C	-0.82869500	-0.94824700	-0.03200700
C	0.46253200	-0.50375000	-0.02843600

H	1.52055500	4.74916800	-0.02199900
H	5.82971900	2.71455200	0.00613800
H	3.94052200	4.29321700	-0.01519800
H	-0.78019100	3.95999900	-0.02309400
H	-1.03934300	-2.01493900	-0.03819200
C	-3.25532000	-0.51794400	-0.02599000
C	-4.34738000	0.35289600	-0.01679600
C	-4.08293600	1.75555200	-0.00851500
H	-4.91187800	2.44907100	-0.00561500
C	-2.78880400	2.23111400	-0.01050000
H	-2.65178100	3.30672800	-0.00413600
H	1.26311600	-1.23426100	-0.03282600
H	-3.42136600	-1.58680100	-0.02492900
H	3.09291400	-0.58498400	-0.01252600
C	7.89269500	-0.89628700	-0.17106400
C	6.91058300	-2.04615300	0.21141400
C	-8.08941800	-0.23849700	0.22267000
C	-7.56930200	-1.64601300	-0.20345900
C	-5.71916100	-0.15593300	-0.01022700
C	5.68660400	-0.01059200	0.00926700
N	5.58536300	-1.37118000	-0.03434400
N	7.01457400	0.30652300	0.06398200
N	-6.08748000	-1.46967600	0.01332900
N	-6.85853800	0.59749800	-0.02265200
O	4.51740900	-2.07395000	-0.11414400
O	7.53635900	1.47112100	0.15104700
O	-6.95147100	1.87256400	-0.07447900
O	-5.32053700	-2.49332400	0.05217000
C	6.93652300	-2.42006800	1.70623200
H	6.09849700	-3.09104300	1.91673200
H	7.86730100	-2.93756300	1.95907100
H	6.84151000	-1.54001300	2.35021500
C	9.15199900	-0.79880900	0.69076400
H	9.74785000	-1.71094100	0.57456200
H	9.75555700	0.05244800	0.36727000
H	8.92149300	-0.66229900	1.74961900
C	7.01813000	-3.30974900	-0.64230200
H	8.01037300	-3.75691000	-0.51485100
H	6.26736400	-4.03540900	-0.32117100
H	6.85807800	-3.10834700	-1.70363600
C	8.27614400	-0.86682800	-1.66358200
H	8.78620800	0.07714400	-1.87699800
H	8.95577300	-1.69065500	-1.90431900
H	7.39811700	-0.93853600	-2.31327300
C	-9.25980200	0.30364100	-0.59846900
H	-10.13088700	-0.34920200	-0.47297300

H	-9.52303400	1.30389600	-0.24687400
H	-9.02393800	0.37379800	-1.66256000
C	-7.75552500	-1.95457500	-1.70148100
H	-7.19363200	-2.86026400	-1.94792600
H	-8.81168400	-2.12719900	-1.93168100
H	-7.38952800	-1.14000300	-2.33447500
C	-8.40282100	-0.11394400	1.72646000
H	-8.56493100	0.94110000	1.96597200
H	-9.31047100	-0.67080100	1.98043300
H	-7.58127400	-0.48509400	2.34723400
C	-8.08241000	-2.81595500	0.63680100
H	-9.17025800	-2.89557000	0.53218100
H	-7.63152300	-3.74641500	0.28399400
H	-7.83897400	-2.70585000	1.69582800

Diradical 7

C	-3.88356300	0.20297000	-0.08243300
C	-3.74477100	1.56273300	0.20288500
C	-2.48266200	2.19704900	0.18823400
C	-1.28764700	1.44477300	-0.05132100
C	-1.47068900	0.08673600	-0.42884000
C	-2.70970000	-0.51945100	-0.44499800
H	-3.32675400	4.17061100	0.52796500
H	-4.62345100	2.15944000	0.40857800
C	-2.40918400	3.61743800	0.34355500
C	-0.00001000	2.11900700	-0.00003900
H	-0.62532300	-0.49522300	-0.77157500
H	-2.79488800	-1.55559300	-0.74151300
C	-0.00001100	3.53971600	0.00018100
C	-1.21906100	4.26476500	0.19117500
H	-1.17074900	5.35038700	0.23401400
C	1.21903900	4.26482700	-0.19057100
C	2.40917400	3.61755000	-0.34306500
C	2.48265400	2.19711900	-0.18812900
C	1.28762300	1.44475700	0.05109100
C	1.47064600	0.08659400	0.42817100
C	2.70967000	-0.51955800	0.44431700
C	3.88357400	0.20300900	0.08215300
C	3.74478600	1.56284400	-0.20281900
H	2.79493400	-1.55577900	0.74054300
H	0.62525400	-0.49551700	0.77058100
H	4.62345500	2.15963900	-0.40829200
H	1.17072100	5.35046000	-0.23311100
H	3.32675000	4.17078200	-0.52727000

C	6.90494700	-2.07472800	0.36930400
C	7.51503900	-0.81813100	-0.32566100
C	-7.51503400	-0.81805300	0.32557200
C	-6.90493400	-2.07482400	-0.36905900
C	5.19335300	-0.44613100	0.05922100
C	-5.19334500	-0.44617300	-0.05940000
N	-6.39235700	0.17220800	0.14146500
N	-5.43199100	-1.78003100	-0.23015100
N	5.43198500	-1.77992500	0.23044600
N	6.39236400	0.17216200	-0.14192500
O	4.57144500	-2.70942700	0.40708400
O	6.60360000	1.42184800	-0.31995800
O	-6.60362100	1.42195900	0.31893600
O	-4.57143400	-2.70963500	-0.40621100
C	7.18849100	-2.15579100	1.88189900
H	6.55923300	-2.93829600	2.31619400
H	8.23684700	-2.41203000	2.06591000
H	6.96556800	-1.21299600	2.39133600
C	8.79616600	-0.27522600	0.30842000
H	9.59206400	-1.02433800	0.23021700
H	9.11437200	0.62523900	-0.22204900
H	8.66176100	-0.01462200	1.36050400
C	7.23252300	-3.41341000	-0.29278700
H	8.31356300	-3.58798400	-0.25399100
H	6.73143500	-4.22148100	0.24521400
H	6.90761900	-3.45286800	-1.33475500
C	7.70934100	-0.97447200	-1.84634100
H	7.94326800	0.00506800	-2.27359400
H	8.53927100	-1.65472300	-2.06273100
H	6.80858600	-1.35664900	-2.33689800
C	-8.79619800	-0.27532200	-0.30856700
H	-9.59210200	-1.02440200	-0.23011500
H	-9.11436600	0.62528500	0.22168900
H	-8.66185800	-0.01498800	-1.36072600
C	-7.18838100	-2.15616400	-1.88166500
H	-6.55917500	-2.93882400	-2.31575800
H	-8.23675400	-2.41232900	-2.06568400
H	-6.96532300	-1.21348700	-2.39125800
C	-7.70920800	-0.97397400	1.84630500
H	-7.94306800	0.00568100	2.27333500
H	-8.53914200	-1.65413800	2.06296200
H	-6.80842700	-1.35606100	2.33688700
C	-7.23264800	-3.41333400	0.29329100
H	-8.31370800	-3.58779400	0.25449900
H	-6.73163500	-4.22157500	-0.24452300
H	-6.90777800	-3.45262300	1.33527700

Optimized coordinate of the diradicals

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

Diradicals-1

C	-3.65818	2.21781	0.00252
C	-1.22152	0.79958	0.00132
C	-1.21958	2.24011	-0.00120
C	-2.48121	2.90723	-0.00554
C	-3.66906	0.77727	0.00948
C	-2.46130	0.10116	0.00231
H	-4.59901	2.74562	0.01741
H	-2.49563	3.99212	-0.01137
C	-4.93289	0.04662	0.00697
H	-2.44986	-0.97836	-0.01654
N	-5.08259	-1.28593	-0.23193
N	-6.16813	0.57781	0.23760
C	-7.26982	-0.40641	-0.07669
C	-6.49283	-1.75364	0.03682
O	-4.17042	-2.13011	-0.50877
O	-6.45088	1.77832	0.55205
C	-7.74590	-0.07507	-1.50192
C	-8.41959	-0.22685	0.91141
C	-6.48238	-2.35447	1.45327
C	-6.88192	-2.82382	-0.98020
H	-6.94420	-0.18530	-2.23472
H	-8.57561	-0.72214	-1.79314
H	-8.09085	0.96007	-1.52306
H	-8.84846	0.76786	0.79189
H	-9.19738	-0.96758	0.70934
H	-8.09722	-0.33017	1.94669
H	-6.20025	-1.61706	2.20736
H	-7.46409	-2.75716	1.70982
H	-5.75633	-3.16864	1.48160
H	-6.23962	-3.69496	-0.85329
H	-7.91843	-3.12883	-0.81585
H	-6.77685	-2.47698	-2.00741

C	0.00000	2.92362	0.00001
C	1.21958	2.24011	0.00120
C	1.22152	0.79958	-0.00132
C	0.00000	0.11507	-0.00000
C	2.46130	0.10116	-0.00231
C	3.65818	2.21781	-0.00252
C	2.48121	2.90723	0.00555
H	2.44986	-0.97836	0.01653
H	2.49563	3.99212	0.01138
H	0.00000	4.00933	0.00001
H	0.00000	-0.97016	-0.00001
C	3.66906	0.77727	-0.00948
C	4.93289	0.04662	-0.00697
N	6.16813	0.57781	-0.23761
N	5.08259	-1.28593	0.23193
C	6.49283	-1.75364	-0.03682
C	7.26982	-0.40641	0.07669
O	6.45088	1.77831	-0.55207
O	4.17042	-2.13011	0.50878
C	8.41959	-0.22685	-0.91141
C	7.74590	-0.07506	1.50191
C	6.48238	-2.35448	-1.45326
C	6.88192	-2.82382	0.98021
H	8.09722	-0.33018	-1.94670
H	8.84846	0.76786	-0.79190
H	9.19738	-0.96759	-0.70934
H	8.57562	-0.72213	1.79314
H	8.09085	0.96008	1.52305
H	6.94420	-0.18529	2.23471
H	6.20025	-1.61707	-2.20735
H	7.46409	-2.75717	-1.70981
H	5.75633	-3.16865	-1.48159
H	6.23962	-3.69496	0.85330
H	7.91844	-3.12882	0.81586
H	6.77686	-2.47697	2.00741
H	4.59901	2.74562	-0.01740

Diradical-2

C	3.70035	2.44730	-0.05144
C	2.64477	3.32750	-0.07156
C	1.30428	2.88448	-0.06070
C	1.04455	1.48563	-0.03741
C	2.13399	0.59504	-0.02066
C	3.45647	1.04630	-0.02310
H	0.43842	4.87432	-0.08875
H	4.71621	2.80936	-0.04383
H	2.84089	4.39445	-0.09139
C	0.21375	3.81313	-0.07108
C	-0.33514	1.02235	-0.03287

H	1.96231	-0.46785	-0.01546
C	-1.38718	1.97910	-0.03695
C	-1.07347	3.38033	-0.05700
H	-1.89407	4.08973	-0.06292
C	-2.73125	1.55951	-0.02600
C	-3.07049	0.20539	-0.01410
C	-2.01414	-0.74729	-0.01717
H	-2.25281	-1.79878	-0.00760
C	-0.69821	-0.34170	-0.02582
H	0.06731	-1.10681	-0.02934
H	-3.51147	2.30519	-0.03316
C	-6.40781	-1.59408	-0.18873
C	-6.83939	-0.15779	0.23181
C	6.77581	-0.79034	-0.09331
C	5.77110	-1.95477	0.15728
C	-4.46830	-0.22123	-0.00106
C	4.56470	0.09386	-0.00080
N	5.88446	0.40395	0.15198
N	4.46171	-1.25907	-0.12774
N	-5.55581	0.60039	-0.00900
N	-4.91492	-1.51055	0.02354
O	-4.21880	-2.57535	0.06196
O	-5.56769	1.87312	-0.05068
O	6.39631	1.55462	0.33665
O	3.40399	-1.94460	-0.31291
C	-6.61185	-1.89656	-1.68354
H	-6.10430	-2.83228	-1.92344
H	-7.67326	-2.00851	-1.91324
H	-6.19890	-1.10955	-2.31757
C	-7.96496	0.45910	-0.59518
H	-8.88366	-0.11555	-0.45316
H	-8.14042	1.48176	-0.26212
H	-7.73076	0.48842	-1.65860
C	-6.98530	-2.72762	0.65548
H	-8.07076	-2.76141	0.53321
H	-6.56865	-3.67710	0.32016
H	-6.75498	-2.61562	1.71423
C	-7.14827	-0.00802	1.73181
H	-7.23230	1.05451	1.96584
H	-8.09318	-0.49370	1.98331
H	-6.36003	-0.43530	2.35472
C	5.92294	-3.16397	-0.76286
H	6.89223	-3.63852	-0.59030
H	5.13863	-3.88784	-0.54280
H	5.84587	-2.89693	-1.81613
C	7.25259	-0.67596	-1.55160
H	7.78071	0.27125	-1.67306
H	7.93820	-1.48868	-1.79901
H	6.41841	-0.69672	-2.25553
C	7.97381	-0.74246	0.85183
H	8.59681	-1.62746	0.70063
H	8.57070	0.14318	0.63535
H	7.67534	-0.69803	1.89838

C	5.69867	-2.41688	1.62333
H	4.83471	-3.07308	1.73993
H	6.59620	-2.97415	1.89853
H	5.58607	-1.57565	2.31007

Diradical-3

C	-1.23213	-0.02272	-0.00315
C	-0.00000	0.65901	0.00000
C	-0.00000	2.11013	-0.00000
C	-1.23478	2.78955	0.00137
C	-2.44483	2.10671	-0.00010
C	1.23212	-0.02272	0.00315
C	1.23478	2.78955	-0.00137
C	2.44483	2.10671	0.00009
C	2.44653	0.66031	0.00582
C	3.68990	-0.03785	0.01030
H	3.67827	-1.11736	-0.00496
C	4.89611	0.63689	0.01602
C	4.88562	2.08233	0.00392
C	3.71221	2.77180	-0.00591
H	1.23409	-1.10810	0.00393
H	-1.23410	-1.10810	-0.00392
H	-1.23682	3.87521	0.00422
H	1.23683	3.87520	-0.00422
H	5.82735	2.60837	0.01570
H	3.72768	3.85667	-0.01538
C	-3.71221	2.77180	0.00590
C	-4.88562	2.08234	-0.00392
H	-5.82735	2.60838	-0.01569
C	-4.89612	0.63691	-0.01602
C	-3.68991	-0.03784	-0.01030
H	-3.67828	-1.11735	0.00496
H	-3.72767	3.85668	0.01538
C	-2.44654	0.66031	-0.00582
C	8.49591	-0.54595	-0.09154
C	7.72187	-1.89174	0.05316
C	-8.49591	-0.54596	0.09154
C	-7.72186	-1.89174	-0.05316
C	6.15918	-0.09298	0.01389
C	-6.15919	-0.09297	-0.01389
N	-7.39781	0.44188	-0.22269
N	-6.30800	-1.42952	0.20496
N	7.39781	0.44188	0.22269
N	6.30801	-1.42953	-0.20496
O	5.39350	-2.27952	-0.45591
O	7.68449	1.64614	0.51828
O	-7.68451	1.64613	-0.51828
O	-5.39348	-2.27951	0.45590
C	7.73145	-2.46985	1.47896
H	7.01027	-3.28732	1.52934

H	8.71849	-2.86298	1.72983
H	7.45456	-1.72191	2.22457
C	9.65881	-0.35037	0.87809
H	10.43407	-1.09418	0.67759
H	10.08578	0.64232	0.73702
H	9.35027	-0.43708	1.91911
C	8.09924	-2.97731	-0.95178
H	9.13743	-3.28037	-0.79446
H	7.45809	-3.84610	-0.80460
H	7.98290	-2.64589	-1.98282
C	8.95266	-0.23591	-1.52794
H	9.29612	0.79914	-1.56929
H	9.77929	-0.88650	-1.82005
H	8.14152	-0.35813	-2.24834
C	-8.09922	-2.97732	0.95178
H	-9.13740	-3.28039	0.79445
H	-7.45806	-3.84611	0.80459
H	-7.98288	-2.64590	1.98282
C	-8.95267	-0.23592	1.52795
H	-9.29613	0.79912	1.56929
H	-9.77928	-0.88653	1.82006
H	-8.14152	-0.35813	2.24835
C	-9.65881	-0.35039	-0.87809
H	-10.43406	-1.09421	-0.67759
H	-10.08579	0.64230	-0.73701
H	-9.35027	-0.43709	-1.91911
C	-7.73144	-2.46986	-1.47896
H	-7.01026	-3.28732	-1.52934
H	-8.71847	-2.86298	-1.72983
H	-7.45455	-1.72190	-2.22457

Diradical-4

C	4.83643	2.17657	-0.06348
C	3.76820	3.02741	-0.09980
C	2.42915	2.54327	-0.08489
C	2.22252	1.12557	-0.04389
C	3.34479	0.25686	-0.01727
C	4.63914	0.75417	-0.01798
C	1.30904	3.38518	-0.10685
C	0.90745	0.62273	-0.03286
C	-0.20586	1.45651	-0.05390
C	0.01048	2.88142	-0.08992
C	-1.12388	3.76720	-0.10635
H	-0.93835	4.83575	-0.13313
C	-2.39034	3.29023	-0.08711
C	-1.57782	0.95248	-0.04021
H	1.45635	4.46048	-0.13574
H	5.84305	2.56456	-0.05363
H	3.93596	4.09877	-0.13492
H	3.18054	-0.81053	-0.01039
H	0.78562	-0.45292	-0.00519

H	-3.23590	3.96953	-0.09790
C	-1.89854	-0.41905	-0.01538
C	-3.20212	-0.86934	-0.00149
H	-3.40647	-1.92786	0.01962
C	-4.28534	0.04802	-0.00936
C	-3.98579	1.41386	-0.03611
H	-4.78915	2.13447	-0.04804
H	-1.11015	-1.16063	-0.00725
C	-2.65827	1.87383	-0.05342
C	-7.56891	-1.84780	-0.17880
C	-8.03846	-0.43159	0.26853
C	8.03547	-0.92893	-0.00605
C	7.07299	-2.15192	0.08818
C	-5.66931	-0.42027	0.01008
C	5.78561	-0.14952	0.01183
C	-7.78113	-2.13377	-1.67570
H	-7.24867	-3.05000	-1.93593
H	-8.84133	-2.27402	-1.89517
H	-7.39944	-1.32505	-2.30199
C	-9.19113	0.16385	-0.53676
H	-10.09076	-0.43998	-0.39367
H	-9.39302	1.17566	-0.18599
H	-8.96984	0.21621	-1.60204
C	-8.10224	-3.01068	0.65460
H	-9.18739	-3.07639	0.54307
H	-7.66018	-3.94187	0.30100
H	-7.86419	-2.90695	1.71251
C	-8.33553	-0.31414	1.77380
H	-8.44983	0.74153	2.02534
H	-9.26222	-0.83275	2.02720
H	-7.52792	-0.72627	2.38193
C	8.59476	-0.67759	-1.41760
H	9.07878	0.30039	-1.43194
H	9.33654	-1.43425	-1.68053
H	7.80848	-0.68241	-2.17501
C	7.33432	-3.27209	-0.91558
H	8.30628	-3.72914	-0.71370
H	6.56374	-4.03594	-0.81344
H	7.32048	-2.91795	-1.94549
C	9.17080	-0.90481	1.01492
H	9.84012	-1.75125	0.84206
H	9.74067	0.01698	0.90085
H	8.80781	-0.94839	2.04105
C	6.93863	-2.73763	1.50463
H	6.10777	-3.44507	1.51205
H	7.84815	-3.26881	1.79185
H	6.73737	-1.96404	2.24829
O	7.51700	1.35461	0.59105
O	4.73423	-2.19780	-0.51865
O	-5.34744	-2.76571	0.02661
O	-6.83085	1.64085	0.00813
N	-6.07664	-1.72243	0.01781
N	-6.78099	0.36862	0.02647

N	5.75032	-1.49090	-0.21980
N	7.07632	0.20362	0.27301

Diradical-5

C	2.20845	0.21117	-0.01188
C	3.53343	0.65395	-0.00485
C	3.76866	2.05024	-0.01440
H	4.78076	2.42229	0.00080
C	2.70714	2.92723	-0.02843
C	1.36386	2.49619	-0.02994
C	1.11910	1.10022	-0.02276
H	2.93522	3.98391	-0.03367
C	0.24584	3.43978	-0.03562
C	-1.08804	2.95608	-0.02606
C	-1.34189	1.51027	-0.01945
C	-0.25670	0.60017	-0.02692
C	0.45931	4.83556	-0.04867
C	-0.59161	5.73125	-0.05098
H	-0.39513	6.79730	-0.06134
C	-1.90724	5.25353	-0.04015
H	-2.74143	5.94590	-0.04193
C	-2.14401	3.89241	-0.02796
H	-3.16988	3.55118	-0.02148
H	1.46697	5.22707	-0.05721
C	-2.65543	1.00947	-0.01112
C	-2.93324	-0.36048	-0.01534
C	-1.84051	-1.26122	-0.03290
H	-2.02221	-2.32389	-0.03749
C	-0.55051	-0.77958	-0.03753
H	-3.49150	1.68564	-0.00613
H	0.25189	-1.50422	-0.05186
H	2.03810	-0.85074	-0.01710
C	6.84897	-1.18605	-0.10927
C	5.84659	-2.34877	0.16031
C	-6.19363	-2.29433	-0.20640
C	-6.68255	-0.88651	0.24658
C	4.63992	-0.29998	0.00862
C	-4.31286	-0.84294	-0.00324
N	-4.70406	-2.15065	-0.00377
N	-5.43461	-0.06908	0.01376
N	4.53345	-1.65332	-0.10779
N	5.96156	0.01040	0.13988
C	-6.39730	-2.57544	-1.70542
H	-5.85247	-3.48359	-1.96841
H	-7.45491	-2.72798	-1.92912
H	-6.02374	-1.75896	-2.32651
C	-7.83972	-0.30172	-0.56013
H	-8.73163	-0.91860	-0.42460
H	-8.05689	0.70509	-0.20424
H	-7.61444	-0.24001	-1.62406

C	-6.71469	-3.46823	0.61934
H	-7.79847	-3.54784	0.50352
H	-6.25898	-4.39169	0.26281
H	-6.48172	-3.36673	1.67860
C	-6.98717	-0.78135	1.75124
H	-7.11705	0.27117	2.00827
H	-7.90758	-1.31422	1.99781
H	-6.17640	-1.18584	2.36026
C	7.30842	-1.07964	-1.57373
H	7.83593	-0.13357	-1.70614
H	7.99027	-1.89428	-1.82513
H	6.46597	-1.10300	-2.26765
C	5.98381	-3.56130	-0.75777
H	6.95426	-4.03741	-0.59646
H	5.20088	-4.28262	-0.52484
H	5.89351	-3.29735	-1.81076
C	8.05827	-1.13379	0.82114
H	8.67927	-2.01964	0.66677
H	8.65271	-0.24936	0.59313
H	7.77235	-1.08426	1.87095
C	5.79537	-2.80600	1.62877
H	4.93382	-3.46265	1.75969
H	6.69730	-3.36146	1.89292
H	5.69146	-1.96281	2.31446
O	-3.96154	-3.18402	0.00411
O	-5.50364	1.20355	0.00152
O	6.47571	1.16301	0.30492
O	3.47186	-2.33873	-0.27041

Diradical-6

C	4.80282	2.34039	-0.04649
C	3.74426	3.21322	-0.07014
C	2.40468	2.76080	-0.06321
C	2.14651	1.36128	-0.04075
C	3.24577	0.47755	-0.02032
C	4.56359	0.93646	-0.01840
C	1.31027	3.67121	-0.07666
C	0.77220	0.89007	-0.04067
C	-0.28872	1.82719	-0.04611
C	0.02368	3.22266	-0.06556
C	-1.66040	1.36151	-0.03604
C	-1.92372	-0.03674	-0.03094
C	-0.82621	-0.94921	-0.03345
C	0.46108	-0.50588	-0.03649
H	1.51733	4.73598	-0.09456
H	5.81718	2.70640	-0.03583
H	3.93234	4.28162	-0.08971
H	-0.77822	3.94834	-0.07508
H	-1.03674	-2.01321	-0.03287

C	-3.24908	-0.51789	-0.02225
C	-4.33758	0.35215	-0.01554
C	-4.07258	1.75220	-0.01819
H	-4.90002	2.44369	-0.01594
C	-2.78181	2.22546	-0.02889
H	-2.64248	3.29820	-0.03092
H	1.26099	-1.23359	-0.04088
H	-3.41659	-1.58399	-0.01424
H	3.08641	-0.58652	-0.01604
C	7.89252	-0.88322	-0.08098
C	6.89308	-2.05410	0.16001
C	-8.07691	-0.23821	0.24848
C	-7.56192	-1.64131	-0.19075
C	-5.70820	-0.15478	-0.00117
C	5.67626	-0.01117	0.00668
N	5.58104	-1.36392	-0.12635
N	6.99396	0.30495	0.16725
N	-6.07528	-1.46751	0.00961
N	-6.84450	0.60056	0.00651
O	4.52758	-2.05483	-0.31761
O	7.49895	1.45689	0.36154
O	-6.93612	1.86989	-0.02349
O	-5.31227	-2.48682	0.02354
C	6.81787	-2.52393	1.62345
H	5.95673	-3.18487	1.73386
H	7.71716	-3.07823	1.89892
H	6.69897	-1.68664	2.31394
C	9.08699	-0.83403	0.86857
H	9.71481	-1.71528	0.71537
H	9.68040	0.05546	0.65841
H	8.78472	-0.79599	1.91429
C	7.05495	-3.25779	-0.76571
H	8.02645	-3.72747	-0.59230
H	6.27425	-3.98743	-0.55189
H	6.97980	-2.98604	-1.81792
C	8.37364	-0.75884	-1.53702
H	8.89701	0.19183	-1.65190
H	9.06456	-1.56650	-1.78624
H	7.54200	-0.78053	-2.24392
C	-9.24529	0.31695	-0.56287
H	-10.12613	-0.31380	-0.41888
H	-9.47949	1.32383	-0.21809
H	-9.02260	0.37069	-1.62777
C	-7.76107	-1.94091	-1.68668
H	-7.19881	-2.84074	-1.94151
H	-8.81565	-2.11628	-1.90781
H	-7.40407	-1.12323	-2.31590
C	-8.38223	-0.12371	1.75230
H	-8.53295	0.92862	1.99860
H	-9.29161	-0.67231	2.00528
H	-7.56299	-0.50570	2.36451
C	-8.06040	-2.81637	0.64718
H	-9.14247	-2.91797	0.53246

H	-7.58696	-3.73449	0.30006
H	-7.82941	-2.69934	1.70530

Diradical-7

C	-3.87516	0.20320	-0.08046
C	-3.73686	1.55943	0.20586
C	-2.47738	2.19271	0.19137
C	-1.28568	1.44199	-0.04970
C	-1.46786	0.08673	-0.42705
C	-2.70347	-0.51740	-0.44411
H	-3.31808	4.16252	0.53221
H	-4.61390	2.15379	0.41235
C	-2.40315	3.61084	0.34619
C	-0.00001	2.11511	-0.00002
H	-0.62288	-0.49369	-0.76499
H	-2.79001	-1.55082	-0.74079
C	0.00000	3.53228	0.00005
C	-1.21679	4.25606	0.19310
H	-1.16829	5.33891	0.23601
C	1.21680	4.25606	-0.19293
C	2.40316	3.61084	-0.34604
C	2.47737	2.19270	-0.19135
C	1.28565	1.44197	0.04961
C	1.46782	0.08667	0.42682
C	2.70341	-0.51748	0.44389
C	3.87513	0.20315	0.08037
C	3.73684	1.55941	-0.20584
H	2.78994	-1.55092	0.74048
H	0.62282	-0.49379	0.76465
H	4.61389	2.15378	-0.41226
H	1.16832	5.33891	-0.23575
H	3.31810	4.16252	-0.53200
C	6.89536	-2.07325	0.36735
C	7.50529	-0.81708	-0.32426
C	-7.50530	-0.81707	0.32420
C	-6.89531	-2.07332	-0.36722
C	5.18340	-0.44516	0.05815
C	-5.18342	-0.44513	-0.05820
N	-6.37993	0.17387	0.14457
N	-5.42030	-1.77741	-0.23149
N	5.42033	-1.77741	0.23164
N	6.37989	0.17385	-0.14475
O	4.56447	-2.70191	0.41105
O	6.58943	1.41678	-0.32637
O	-6.58952	1.41683	0.32596
O	-4.56439	-2.70191	-0.41072
C	7.17699	-2.15750	1.87780
H	6.54613	-2.93754	2.30729
H	8.22141	-2.41653	2.06262

H	6.95545	-1.21738	2.38669
C	8.78002	-0.26886	0.31290
H	9.58512	-1.00172	0.21688
H	9.07804	0.64350	-0.20319
H	8.64749	-0.02951	1.36727
C	7.21623	-3.40989	-0.29716
H	8.29085	-3.60038	-0.24030
H	6.69382	-4.20975	0.22715
H	6.90960	-3.43817	-1.34199
C	7.70207	-0.97014	-1.84262
H	7.93265	0.00931	-2.26489
H	8.53252	-1.64490	-2.05918
H	6.80489	-1.35255	-2.33321
C	-8.78004	-0.26899	-0.31305
H	-9.58512	-1.00187	-0.21695
H	-9.07811	0.64342	0.20292
H	-8.64751	-0.02977	-1.36745
C	-7.17689	-2.15777	-1.87766
H	-6.54601	-2.93786	-2.30704
H	-8.22131	-2.41685	-2.06247
H	-6.95536	-1.21772	-2.38667
C	-7.70209	-0.96992	1.84259
H	-7.93271	0.00957	2.26471
H	-8.53252	-1.64468	2.05923
H	-6.80490	-1.35224	2.33323
C	-7.21616	-3.40988	0.29746
H	-8.29078	-3.60041	0.24059
H	-6.69371	-4.20980	-0.22672
H	-6.90957	-3.43801	1.34231

BP86/6-311++G(d,p)

Diradical-1

C	-3.67728	2.22381	-0.00415
C	-1.22900	0.79621	0.00187
C	-1.22637	2.24671	-0.00220
C	-2.49049	2.91662	-0.00934
C	-3.68933	0.77851	0.00857
C	-2.47188	0.09552	0.00658

H	-4.62903	2.75265	0.00256
H	-2.50389	4.01077	-0.01686
C	-4.95623	0.04920	0.01036
H	-2.46729	-0.99447	-0.00280
N	-5.10116	-1.31143	-0.11365
N	-6.20962	0.60207	0.13106
C	-7.30065	-0.42255	-0.15521
C	-6.53789	-1.74913	0.14494
O	-4.17860	-2.18625	-0.26530
O	-6.51430	1.83239	0.31061
C	-7.67552	-0.23705	-1.63950
C	-8.51157	-0.13792	0.73497
C	-6.58948	-2.17891	1.62488
C	-6.88039	-2.93101	-0.76320
H	-6.81979	-0.42814	-2.30476
H	-8.49821	-0.91179	-1.92060
H	-8.00802	0.80075	-1.79135
H	-8.90633	0.86056	0.50106
H	-9.29989	-0.88199	0.54026
H	-8.26000	-0.15949	1.80379
H	-6.33709	-1.34685	2.29970
H	-7.59054	-2.55354	1.88714
H	-5.86116	-2.98827	1.78295
H	-6.20795	-3.76955	-0.53408
H	-7.91774	-3.25273	-0.58070
H	-6.76658	-2.68829	-1.82824
C	0.00000	2.93351	0.00001
C	1.22637	2.24670	0.00221
C	1.22899	0.79620	-0.00188
C	-0.00001	0.10836	-0.00001
C	2.47187	0.09551	-0.00660
C	3.67727	2.22378	0.00417
C	2.49049	2.91661	0.00936
H	2.46726	-0.99449	0.00276
H	2.50390	4.01075	0.01690
H	0.00001	4.02860	0.00002
H	-0.00001	-0.98616	-0.00002
C	3.68932	0.77849	-0.00857
C	4.95622	0.04918	-0.01037
N	6.20960	0.60207	-0.13107
N	5.10117	-1.31145	0.11365
C	6.53791	-1.74912	-0.14493
C	7.30065	-0.42253	0.15521
O	6.51425	1.83239	-0.31064
O	4.17863	-2.18628	0.26532
C	8.51156	-0.13789	-0.73498
C	7.67551	-0.23701	1.63949
C	6.58950	-2.17892	-1.62487
C	6.88043	-2.93099	0.76323
H	8.25999	-0.15948	-1.80381
H	8.90630	0.86060	-0.50108
H	9.29989	-0.88194	-0.54027
H	8.49822	-0.91173	1.92060

H	8.00800	0.80081	1.79132
H	6.81979	-0.42811	2.30475
H	6.33709	-1.34688	-2.29970
H	7.59058	-2.55354	-1.88712
H	5.86121	-2.98830	-1.78293
H	6.20800	-3.76954	0.53412
H	7.91779	-3.25269	0.58073
H	6.76662	-2.68826	1.82826
H	4.62903	2.75262	-0.00253

Diradical-2

C	3.72037	2.45668	-0.04647
C	2.65928	3.34347	-0.06593
C	1.31153	2.90025	-0.05888
C	1.04820	1.49090	-0.03974
C	2.14097	0.59513	-0.02433
C	3.47198	1.04948	-0.02304
H	0.44723	4.90191	-0.08315
H	4.74846	2.81483	-0.03447
H	2.85714	4.41959	-0.08224
C	0.21939	3.83190	-0.06802
C	-0.33545	1.02828	-0.03673
H	1.97202	-0.47952	-0.02359
C	-1.39484	1.99305	-0.03879
C	-1.07896	3.39734	-0.05617
H	-1.90588	4.11349	-0.06123
C	-2.74515	1.57150	-0.02808
C	-3.08443	0.20804	-0.01783
C	-2.02409	-0.75024	-0.02337
H	-2.27126	-1.81039	-0.01447
C	-0.70025	-0.34177	-0.03214
H	0.07353	-1.11212	-0.03735
H	-3.53702	2.32036	-0.03440
C	-6.43582	-1.59952	-0.19348
C	-6.86815	-0.16501	0.23950
C	6.80165	-0.80249	-0.10101
C	5.79552	-1.96459	0.16688
C	-4.48275	-0.22071	-0.00362
C	4.58028	0.09540	-0.00125
N	5.90995	0.40759	0.15182
N	4.47356	-1.26816	-0.12866
N	-5.57901	0.60717	-0.01254
N	-4.92970	-1.52055	0.02426
O	-4.23111	-2.59247	0.06173
O	-5.59480	1.88696	-0.05389
O	6.42982	1.56347	0.33147
O	3.40999	-1.95902	-0.31027
C	-6.63182	-1.88596	-1.69599
H	-6.11535	-2.82485	-1.94566
H	-7.70024	-2.00008	-1.93409

H	-6.21488	-1.08289	-2.32262
C	-8.00186	0.45885	-0.57588
H	-8.93488	-0.10093	-0.40540
H	-8.15202	1.49794	-0.25117
H	-7.78641	0.46854	-1.65272
C	-7.01039	-2.74432	0.64238
H	-8.10040	-2.80143	0.49588
H	-6.56217	-3.69237	0.31379
H	-6.80257	-2.62512	1.71417
C	-7.15618	-0.02269	1.74780
H	-7.23428	1.04778	1.99010
H	-8.10673	-0.51048	2.01216
H	-6.35347	-0.45955	2.36119
C	5.93975	-3.18767	-0.74050
H	6.90137	-3.68697	-0.54289
H	5.12725	-3.89588	-0.52627
H	5.88850	-2.92678	-1.80610
C	7.25651	-0.69121	-1.56998
H	7.78458	0.26498	-1.70262
H	7.94619	-1.50915	-1.82780
H	6.40369	-0.71640	-2.26523
C	8.01097	-0.74756	0.83332
H	8.65785	-1.62081	0.65542
H	8.58795	0.16431	0.62525
H	7.72095	-0.73059	1.89229
C	5.71922	-2.40267	1.64366
H	4.84449	-3.05795	1.77000
H	6.62035	-2.96465	1.93226
H	5.60830	-1.54180	2.32047

Diradical-3

C	-1.23754	-0.02919	-0.00311
C	0.00000	0.65552	0.00000
C	0.00000	2.11670	0.00001
C	-1.23963	2.79922	0.00395
C	-2.45818	2.11288	0.00426
C	1.23754	-0.02919	0.00310
C	1.23963	2.79922	-0.00394
C	2.45818	2.11287	-0.00424
C	2.46077	0.65750	0.00413
C	3.70642	-0.04281	0.01114
H	3.70172	-1.13284	0.00456
C	4.92211	0.63912	0.01054
C	4.91072	2.08831	-0.00792
C	3.72696	2.78126	-0.01471
H	1.23984	-1.12389	0.00552
H	-1.23984	-1.12389	-0.00553
H	-1.24168	3.89424	0.00771
H	1.24168	3.89424	-0.00769

H	5.86329	2.61565	-0.00405
H	3.74110	3.87537	-0.02662
C	-3.72696	2.78126	0.01473
C	-4.91072	2.08831	0.00793
H	-5.86329	2.61565	0.00407
C	-4.92211	0.63912	-0.01054
C	-3.70642	-0.04281	-0.01114
H	-3.70172	-1.13284	-0.00457
H	-3.74110	3.87537	0.02664
C	-2.46077	0.65750	-0.00413
C	8.53252	-0.56190	-0.15600
C	7.76995	-1.88879	0.14348
C	-8.53252	-0.56190	0.15598
C	-7.76995	-1.88879	-0.14348
C	6.18818	-0.08993	0.01263
C	-6.18818	-0.08993	-0.01263
N	-7.44227	0.46238	-0.13397
N	-6.33320	-1.45063	0.11295
N	7.44227	0.46238	0.13395
N	6.33320	-1.45064	-0.11293
O	5.41009	-2.32516	-0.26443
O	7.74745	1.69176	0.31844
O	-7.74745	1.69176	-0.31848
O	-5.41009	-2.32516	0.26445
C	7.82360	-2.32037	1.62284
H	7.09551	-3.12993	1.78094
H	8.82502	-2.69533	1.88329
H	7.57219	-1.48910	2.29900
C	9.74517	-0.27913	0.73238
H	10.53268	-1.02341	0.53528
H	10.14012	0.71942	0.49913
H	9.49547	-0.30194	1.80162
C	8.11146	-3.06947	-0.76660
H	9.14933	-3.39079	-0.58636
H	7.43997	-3.90872	-0.53730
H	7.99559	-2.82557	-1.83115
C	8.90476	-0.37429	-1.64073
H	9.23737	0.66363	-1.79163
H	9.72679	-1.04880	-1.92434
H	8.04780	-0.56412	-2.30477
C	-8.11146	-3.06946	0.76663
H	-9.14933	-3.39079	0.58638
H	-7.43997	-3.90871	0.53733
H	-7.99560	-2.82554	1.83117
C	-8.90478	-0.37427	1.64071
H	-9.23739	0.66365	1.79159
H	-9.72681	-1.04878	1.92432
H	-8.04782	-0.56409	2.30476
C	-9.74516	-0.27914	-0.73241
H	-10.53267	-1.02342	-0.53531
H	-10.14012	0.71941	-0.49917
H	-9.49546	-0.30197	-1.80165
C	-7.82359	-2.32039	-1.62283

H	-7.09550	-3.12995	-1.78091
H	-8.82500	-2.69536	-1.88328
H	-7.57218	-1.48913	-2.29899

Diradical-4

C	4.86093	2.18478	-0.05209
C	3.78513	3.04241	-0.08290
C	2.44149	2.55747	-0.07463
C	2.23216	1.12901	-0.04569
C	3.35640	0.25618	-0.02363
C	4.66100	0.75749	-0.01825
C	1.31671	3.40420	-0.09120
C	0.90993	0.62559	-0.03964
C	-0.20977	1.46523	-0.05425
C	0.00878	2.89898	-0.07927
C	-1.12616	3.78734	-0.08946
H	-0.93815	4.86501	-0.10867
C	-2.40399	3.30743	-0.07340
C	-1.58400	0.96023	-0.04378
H	1.46564	4.48895	-0.11144
H	5.87912	2.57061	-0.03649
H	3.95449	4.12312	-0.10870
H	3.19554	-0.82220	-0.02479
H	0.78537	-0.45976	-0.02002
H	-3.25627	3.99310	-0.07918
C	-1.90586	-0.41825	-0.02857
C	-3.21667	-0.87238	-0.01571
H	-3.42862	-1.94006	-0.00036
C	-4.30505	0.05003	-0.01540
C	-4.00664	1.42516	-0.03383
H	-4.82216	2.14816	-0.04085
H	-1.10872	-1.16469	-0.02675
C	-2.67290	1.88854	-0.04952
C	-7.60166	-1.85607	-0.18560
C	-8.07233	-0.44119	0.27177
C	8.06753	-0.94414	-0.03550
C	7.10341	-2.16184	0.11784
C	-5.68922	-0.42094	0.00441
C	5.80783	-0.14796	0.00909
C	-7.80626	-2.12818	-1.68956
H	-7.26516	-3.04776	-1.95817
H	-8.87356	-2.27076	-1.91710
H	-7.42075	-1.30458	-2.30968
C	-9.23287	0.15958	-0.52316
H	-10.14720	-0.42956	-0.35036
H	-9.40965	1.18941	-0.18273
H	-9.02963	0.18986	-1.60197
C	-8.13123	-3.02885	0.64123
H	-9.22030	-3.11918	0.50487

H	-7.65646	-3.95795	0.29618
H	-7.91633	-2.91654	1.71238
C	-8.34928	-0.32861	1.78464
H	-8.45967	0.73526	2.04287
H	-9.28077	-0.85078	2.05106
H	-7.52679	-0.74757	2.38413
C	8.58123	-0.72789	-1.47335
H	9.06603	0.25838	-1.52828
H	9.32224	-1.49565	-1.74294
H	7.76297	-0.75380	-2.20904
C	7.34266	-3.32061	-0.85108
H	8.30893	-3.79968	-0.62828
H	6.54502	-4.06657	-0.72730
H	7.34171	-2.99647	-1.90033
C	9.23165	-0.89206	0.95506
H	9.92206	-1.72824	0.76298
H	9.77847	0.05168	0.82091
H	8.89585	-0.94219	1.99944
C	6.98181	-2.68997	1.56164
H	6.13301	-3.38845	1.60912
H	7.89396	-3.22903	1.85946
H	6.80292	-1.87612	2.28077
O	7.56968	1.37248	0.52731
O	4.73997	-2.22249	-0.46777
O	-5.36346	-2.78374	0.02601
O	-6.86483	1.65261	-0.00192
N	-6.09598	-1.73395	0.01653
N	-6.81008	0.37349	0.01818
N	5.76553	-1.50462	-0.19840
N	7.11302	0.21062	0.24414

Diradical-5

C	2.21588	0.20817	-0.01702
C	3.54869	0.65461	-0.00162
C	3.78765	2.05790	-0.00082
H	4.81170	2.42662	0.02303
C	2.72023	2.94039	-0.01486
C	1.37006	2.50831	-0.02593
C	1.12220	1.10217	-0.02660
H	2.94863	4.00708	-0.01216
C	0.25092	3.45422	-0.03416
C	-1.09308	2.96843	-0.03034
C	-1.34917	1.52035	-0.02559
C	-0.25655	0.60286	-0.03512
C	0.46619	4.85658	-0.04552
C	-0.59039	5.75857	-0.05155
H	-0.39124	6.83329	-0.06073
C	-1.91334	5.27954	-0.04682
H	-2.75384	5.97838	-0.05224

C	-2.15282	3.91026	-0.03652
H	-3.18733	3.56430	-0.03568
H	1.48411	5.24872	-0.05040
C	-2.66914	1.01808	-0.01666
C	-2.94716	-0.36072	-0.02297
C	-1.85002	-1.26765	-0.04471
H	-2.04031	-2.33926	-0.05063
C	-0.55250	-0.78343	-0.04945
H	-3.51719	1.69772	-0.00927
H	0.25868	-1.51280	-0.06589
H	2.04838	-0.86563	-0.03040
C	6.87574	-1.19830	-0.11302
C	5.87183	-2.36079	0.16376
C	-6.22243	-2.30278	-0.20625
C	-6.71026	-0.89567	0.25699
C	4.65574	-0.30034	0.01022
C	-4.32729	-0.84496	-0.00764
N	-4.71859	-2.16303	-0.00241
N	-5.45796	-0.06490	0.00869
N	4.54641	-1.66359	-0.11421
N	5.98674	0.01212	0.14752
C	-6.42306	-2.57103	-1.71142
H	-5.87083	-3.48291	-1.98363
H	-7.48847	-2.72554	-1.93998
H	-6.04720	-1.74038	-2.32802
C	-7.87727	-0.30563	-0.53667
H	-8.78405	-0.90773	-0.36874
H	-8.06820	0.71987	-0.19098
H	-7.67248	-0.26687	-1.61490
C	-6.73788	-3.48550	0.61534
H	-7.82549	-3.58972	0.47716
H	-6.25041	-4.40690	0.26737
H	-6.52575	-3.37468	1.68720
C	-6.99074	-0.79391	1.77001
H	-7.11560	0.26707	2.03335
H	-7.91554	-1.32981	2.03240
H	-6.16360	-1.20496	2.36853
C	7.31811	-1.08641	-1.58578
H	7.84563	-0.13044	-1.72214
H	8.00508	-1.90457	-1.85001
H	6.45949	-1.11051	-2.27388
C	6.00476	-3.58146	-0.74863
H	6.96738	-4.08310	-0.56221
H	5.19310	-4.28867	-0.52798
H	5.94323	-3.31738	-1.81288
C	8.09307	-1.14373	0.81084
H	8.73851	-2.01678	0.62697
H	8.66817	-0.23169	0.59822
H	7.81208	-1.12744	1.87223
C	5.81308	-2.80334	1.63999
H	4.94061	-3.46003	1.77435
H	6.71816	-3.36518	1.91616
H	5.70894	-1.94489	2.32089

O	-3.97358	-3.20350	0.00443
O	-5.53091	1.21462	-0.00564
O	6.50767	1.16912	0.31603
O	3.47974	-2.35375	-0.27994

Diradical-6

C	4.82670	2.34884	-0.03693
C	3.76128	3.22727	-0.05994
C	2.41553	2.77306	-0.05991
C	2.15571	1.36262	-0.04496
C	3.25860	0.47514	-0.02605
C	4.58486	0.93879	-0.01715
C	1.31778	3.68600	-0.07254
C	0.77712	0.88990	-0.04918
C	-0.29216	1.83486	-0.05205
C	0.02107	3.23401	-0.06612
C	-1.66782	1.36684	-0.04366
C	-1.93284	-0.04222	-0.04242
C	-0.83164	-0.95707	-0.04839
C	0.46531	-0.50951	-0.05006
H	1.52693	4.75983	-0.08579
H	5.85277	2.71230	-0.01947
H	3.94987	4.30506	-0.07351
H	-0.78885	3.96535	-0.07473
H	-1.04411	-2.03003	-0.05106
C	-3.26376	-0.52507	-0.03335
C	-4.35808	0.35266	-0.02257
C	-4.09296	1.75909	-0.02262
H	-4.93212	2.45269	-0.01825
C	-2.79352	2.23452	-0.03358
H	-2.65071	3.31664	-0.03308
H	1.27380	-1.24210	-0.05643
H	-3.43913	-1.60063	-0.02668
H	3.10328	-0.60099	-0.02892
C	7.92624	-0.89240	-0.08622
C	6.92634	-2.06230	0.17059
C	-8.11138	-0.24307	0.26104
C	-7.59977	-1.64520	-0.19213
C	-5.72988	-0.15407	-0.00485
C	5.69864	-0.00914	0.00739
N	5.60137	-1.37272	-0.12694
N	7.02571	0.31054	0.16900
N	-6.09877	-1.47744	0.00942
N	-6.87353	0.60837	0.00504
O	4.54293	-2.07006	-0.31565
O	7.53749	1.46826	0.35875
O	-6.96842	1.88475	-0.02423
O	-5.33376	-2.50423	0.01891

C	6.84649	-2.50935	1.64448
H	5.97482	-3.17000	1.76359
H	7.74947	-3.06816	1.93346
H	6.72839	-1.65291	2.32567
C	9.13091	-0.83488	0.85390
H	9.78423	-1.70296	0.67431
H	9.70301	0.08173	0.65337
H	8.83607	-0.82547	1.91162
C	7.08281	-3.27912	-0.74326
H	8.04773	-3.77189	-0.54548
H	6.27537	-3.99507	-0.53568
H	7.03283	-3.01278	-1.80758
C	8.38701	-0.77031	-1.55246
H	8.91008	0.18965	-1.67751
H	9.08263	-1.58274	-1.81170
H	7.53747	-0.79660	-2.25167
C	-9.28906	0.32137	-0.53532
H	-10.18621	-0.29284	-0.35968
H	-9.49467	1.34710	-0.19881
H	-9.08715	0.35334	-1.61431
C	-7.79728	-1.92786	-1.69495
H	-7.22917	-2.83161	-1.96157
H	-8.86002	-2.10305	-1.92085
H	-7.43716	-1.09494	-2.31789
C	-8.39139	-0.13439	1.77363
H	-8.53535	0.92623	2.02860
H	-9.30585	-0.68496	2.04179
H	-7.55598	-0.52547	2.37405
C	-8.09393	-2.83035	0.63902
H	-9.17950	-2.95515	0.50196
H	-7.59000	-3.74560	0.29829
H	-7.88371	-2.70698	1.70989

Diradical-7

C	-3.88307	0.20749	-0.08587
C	-3.75150	1.57360	0.20339
C	-2.48937	2.21454	0.18874
C	-1.28713	1.46133	-0.05526
C	-1.46409	0.10138	-0.44054
C	-2.70513	-0.51169	-0.45788
H	-3.34024	4.19103	0.53643
H	-4.64320	2.16531	0.41022
C	-2.41667	3.63688	0.34692
C	-0.00001	2.13720	-0.00008
H	-0.60696	-0.47505	-0.78743
H	-2.79543	-1.55367	-0.76087
C	-0.00004	3.56580	0.00002
C	-1.22202	4.28928	0.19295
H	-1.17484	5.38147	0.23522

C	1.22191	4.28936	-0.19279
C	2.41660	3.63704	-0.34681
C	2.48937	2.21468	-0.18881
C	1.28715	1.46138	0.05503
C	1.46416	0.10138	0.44012
C	2.70523	-0.51162	0.45745
C	3.88316	0.20767	0.08565
C	3.75153	1.57381	-0.20346
H	2.79557	-1.55364	0.76031
H	0.60703	-0.47515	0.78686
H	4.64321	2.16560	-0.41016
H	1.17468	5.38155	-0.23492
H	3.34015	4.19125	-0.53621
C	6.90905	-2.08720	0.37765
C	7.52106	-0.84039	-0.33332
C	-7.52097	-0.84025	0.33352
C	-6.90921	-2.08714	-0.37755
C	5.18916	-0.44736	0.06138
C	-5.18908	-0.44751	-0.06153
N	-6.39682	0.17149	0.14764
N	-5.42041	-1.79040	-0.23935
N	5.42030	-1.79027	0.23925
N	6.39700	0.17150	-0.14765
O	4.55791	-2.71688	0.42800
O	6.61538	1.41891	-0.33849
O	-6.61495	1.41894	0.33854
O	-4.55818	-2.71717	-0.42810
C	7.18726	-2.14694	1.89327
H	6.54365	-2.92081	2.33780
H	8.23732	-2.41367	2.08717
H	6.96978	-1.18798	2.38771
C	8.80684	-0.28939	0.28513
H	9.62542	-1.01423	0.15315
H	9.08024	0.64467	-0.22525
H	8.69628	-0.07050	1.35555
C	7.22065	-3.43705	-0.27044
H	8.29800	-3.64951	-0.18742
H	6.66592	-4.22751	0.25401
H	6.93371	-3.46869	-1.33001
C	7.69209	-1.00659	-1.85677
H	7.92216	-0.02312	-2.29318
H	8.52265	-1.69196	-2.08372
H	6.77714	-1.39154	-2.33213
C	-8.80679	-0.28911	-0.28470
H	-9.62543	-1.01386	-0.15260
H	-9.08000	0.64498	0.22573
H	-8.69640	-0.07021	-1.35515
C	-7.18764	-2.14682	-1.89314
H	-6.54425	-2.92082	-2.33776
H	-8.23779	-2.41334	-2.08689
H	-6.97004	-1.18790	-2.38760
C	-7.69174	-1.00643	1.85699
H	-7.92163	-0.02294	2.29344

H	-8.52234	-1.69171	2.08410
H	-6.77675	-1.39148	2.33219
C	-7.22090	-3.43696	0.27056
H	-8.29830	-3.64928	0.18768
H	-6.66634	-4.22749	-0.25397
H	-6.93383	-3.46865	1.33010