

The supplementary data (ky3061)

(I)

Calculation Method = RB3LYP
Basis Set = 6-311++G(d,p)
Charge = 0
Spin = Singlet
E(RB3LYP) = -517.60718162 a.u.
RMS Gradient Norm = 0.00006726 a.u.
Imaginary Freq = 0
Dipole Moment = 1.6472 Debye
Point Group = C2V
Job cpu time: 0 days 1 hours 20 minutes 49.9 seconds.

C	0.00000000	3.04160400	-1.15245200
C	0.00000000	3.42553300	0.19869200
C	0.00000000	2.47968300	1.21896500
C	0.00000000	1.13288100	0.85492500
C	0.00000000	0.72501600	-0.50375200
C	0.00000000	1.69757900	-1.50893400
H	0.00000000	3.80356500	-1.92302900
H	0.00000000	4.47936800	0.45310800
H	0.00000000	2.78317100	2.26002200
H	0.00000000	1.40890900	-2.55421600
C	0.00000000	-1.13288100	0.85492500
C	0.00000000	-2.47968300	1.21896500
C	0.00000000	-3.42553300	0.19869200
C	0.00000000	-3.04160400	-1.15245200
C	0.00000000	-1.69757900	-1.50893400
C	0.00000000	-0.72501600	-0.50375200
H	0.00000000	-2.78317100	2.26002200
H	0.00000000	-4.47936800	0.45310800
H	0.00000000	-3.80356500	-1.92302900
H	0.00000000	-1.40890900	-2.55421600
N	0.00000000	0.00000000	1.65410800
H	0.00000000	0.00000000	2.66015500

(II)

Calculation Method = RB3LYP
Basis Set = 6-311++G(d,p)
Charge = 0
Spin = Singlet
E(RB3LYP) = -722.17919731 a.u.
RMS Gradient Norm = 0.00004069 a.u.
Imaginary Freq = 0
Dipole Moment = 4.3580 Debye
Point Group = CS
Job cpu time: 0 days 2 hours 58 minutes 41.9 seconds

C	-2.68807300	-1.34008200	0.00000000
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C	-1.68975400	-2.31042400	0.00000000
C	-0.34392700	-1.93898600	0.00000000
C	0.00000000	-0.57864700	0.00000000
C	-1.02840700	0.40969100	0.00000000
C	-2.36350600	0.01949000	0.00000000
H	-3.72618900	-1.64748800	0.00000000
H	-1.93032800	-3.36453900	0.00000000
H	-3.15113800	0.76441400	0.00000000
C	1.03252300	1.42402100	0.00000000
C	1.98421200	2.44194200	0.00000000
C	1.52050000	3.75317900	0.00000000
C	0.14614000	4.04278200	0.00000000
C	-0.79704500	3.02202000	0.00000000
C	-0.35654700	1.69500600	0.00000000
H	3.04542900	2.22268000	0.00000000
H	2.23544500	4.56768000	0.00000000
H	-0.17980300	5.07602600	0.00000000
H	-1.85599900	3.25417000	0.00000000
N	1.21569900	0.04587100	0.00000000
H	2.08628600	-0.46374100	0.00000000
N	0.68412000	-2.96441700	0.00000000
O	1.86326100	-2.58598600	0.00000000
O	0.34684800	-4.14143000	0.00000000

(III)

Calculation Method = RB3LYP

Basis Set = 6-311++G(d,p)

Charge = 0

Spin = Singlet

E(RB3LYP) = -722.14069373 a.u.

RMS Gradient Norm = 0.00005804 a.u.

Imaginary Freq = 0

Dipole Moment = 4.0902 Debye

Point Group = CS

Job cpu time: 0 days 3 hours 38 minutes 8.2 seconds

C	1.88191000	-3.01556700	0.00000000
C	0.54716600	-3.43250200	0.00000000
C	-0.50689300	-2.51902700	0.00000000
C	-0.17952100	-1.16498500	0.00000000
C	1.16148800	-0.72621500	0.00000000
C	2.19642700	-1.66042600	0.00000000
H	2.67530500	-3.75355800	0.00000000
H	0.31721800	-4.49148300	0.00000000
H	-1.53136000	-2.85207400	0.00000000
H	3.22987400	-1.33397100	0.00000000
C	-0.17952800	1.16500500	0.00000000
C	-0.50689500	2.51905000	0.00000000
C	0.54716600	3.43252400	0.00000000
C	1.88191000	3.01558900	0.00000000

C	2.19642400	1.66044800	0.00000000
C	1.16148500	0.72623700	0.00000000
H	-1.53135800	2.85210400	0.00000000
H	0.31721900	4.49150500	0.00000000
H	2.67530500	3.75357900	0.00000000
H	3.22987100	1.33399300	0.00000000
N	-0.99518800	0.00000500	0.00000000
N	-2.38206700	-0.00002600	0.00000000
O	-2.93429600	1.09022400	0.00000000
O	-2.93421900	-1.09031600	0.00000000