A 3,4-Dioxocyclobut-1-ene-1,2-Dithiolate Chelated Ruthenium Carbene Catalyst for Z-Stereoretentive/Stereoselective Olefin Metathesis

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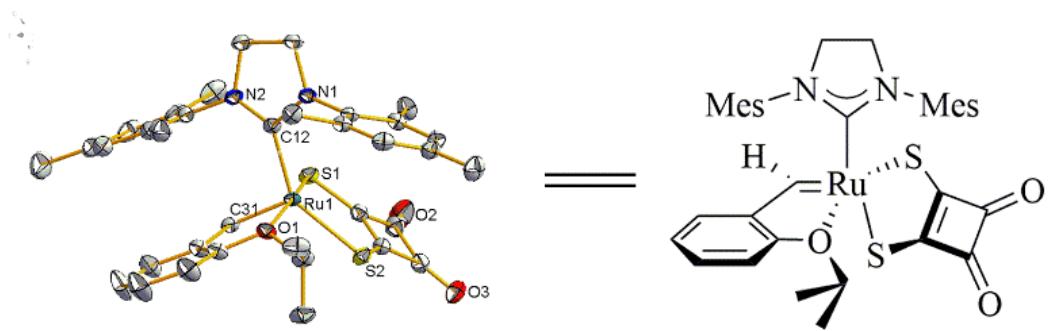
[c] School of Chemical Engineering & Technology, Tianjin University, Tianjin 300350, P. R. China.

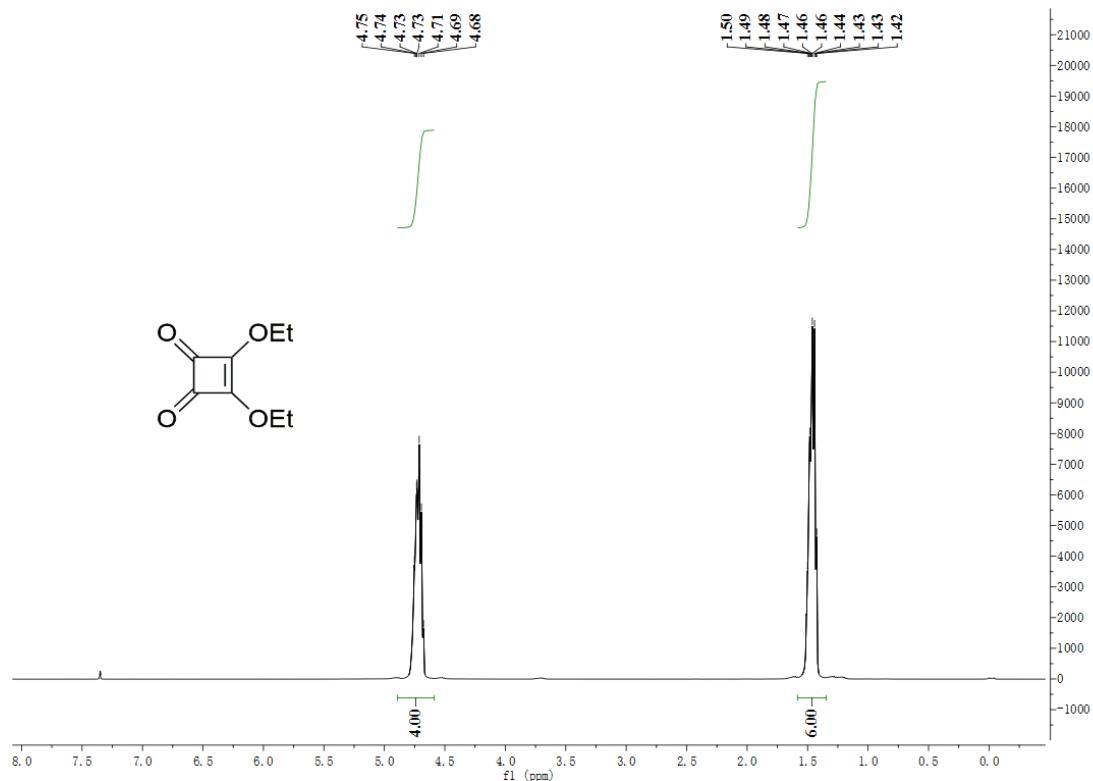[d] College of Chemistry and Molecular Engineering, Peking University, Beijing 100871, China.

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Figure S4. ^{1}H NMR spectrum of **11** in CD$_2$Cl$_2$ (400 Hz)
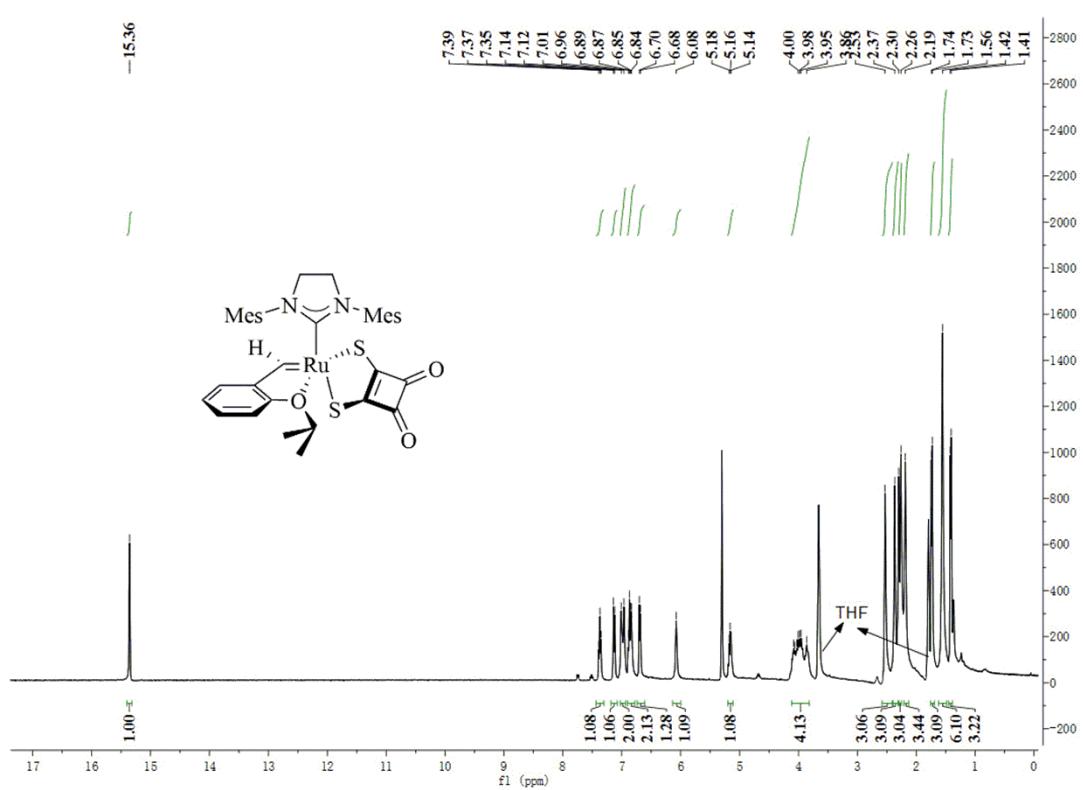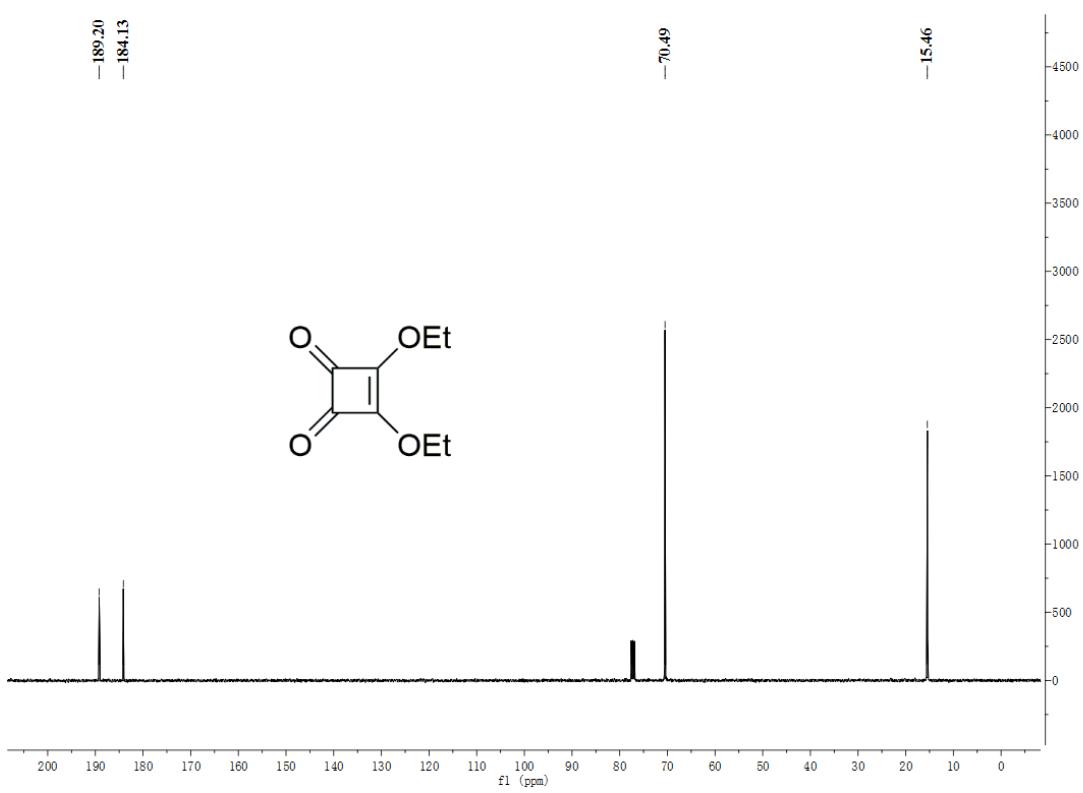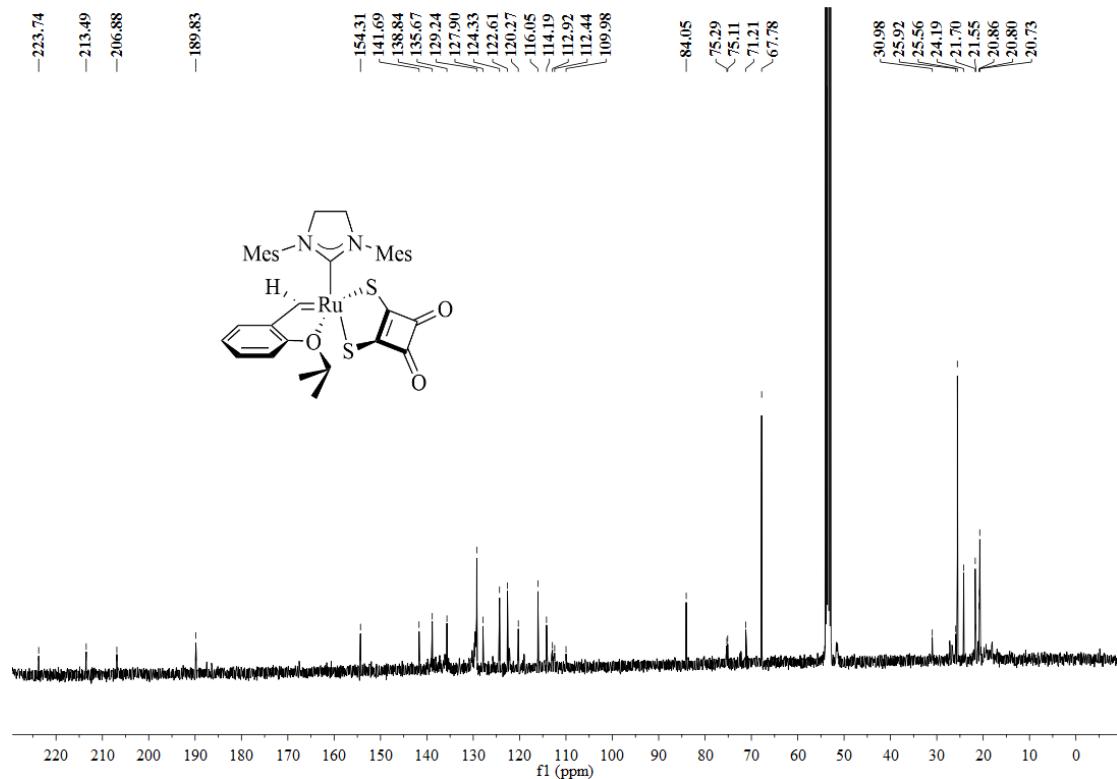
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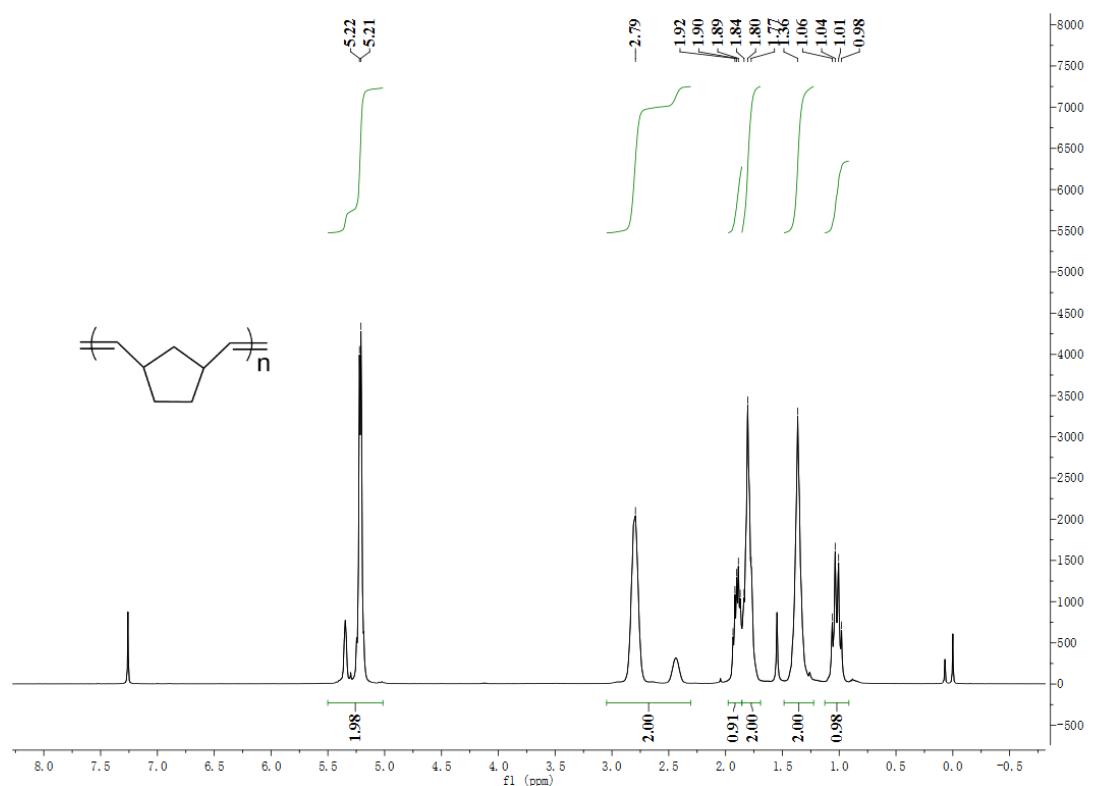
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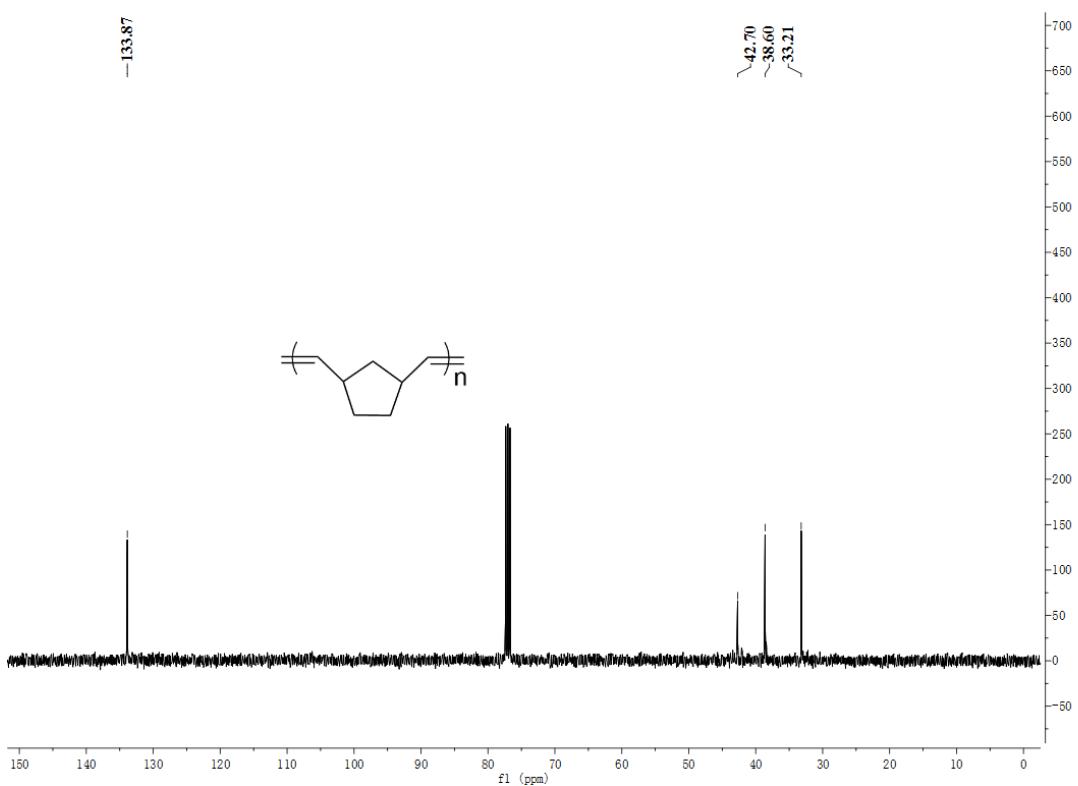
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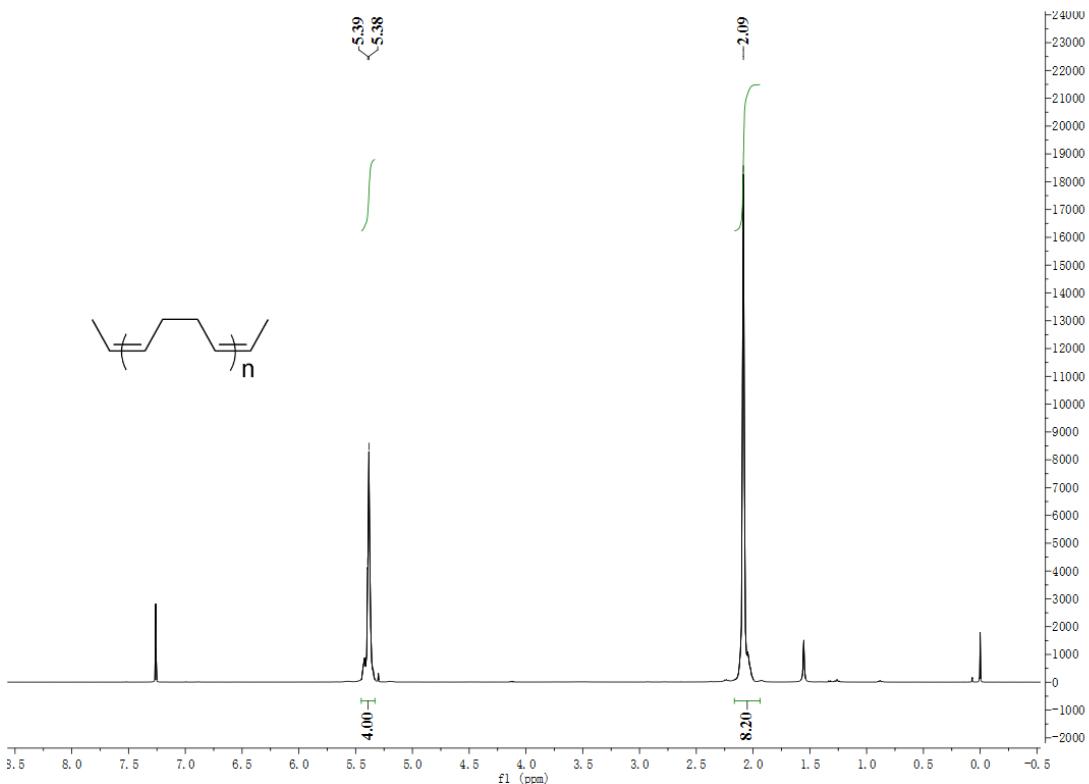
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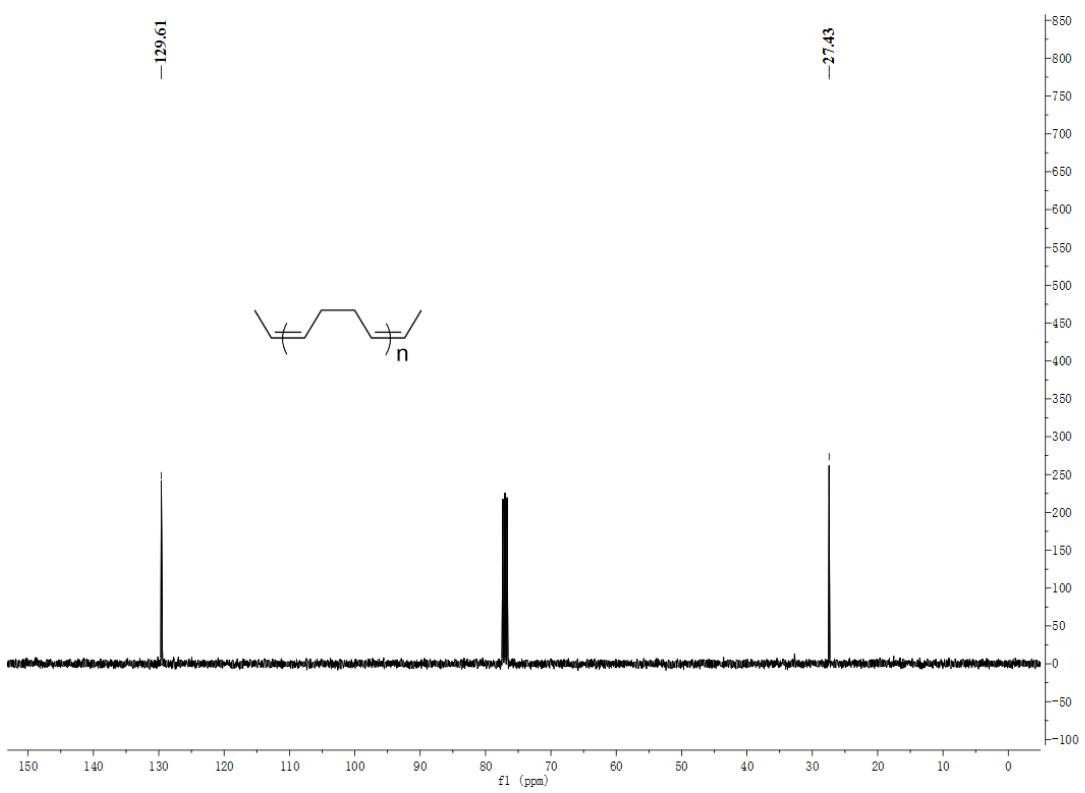
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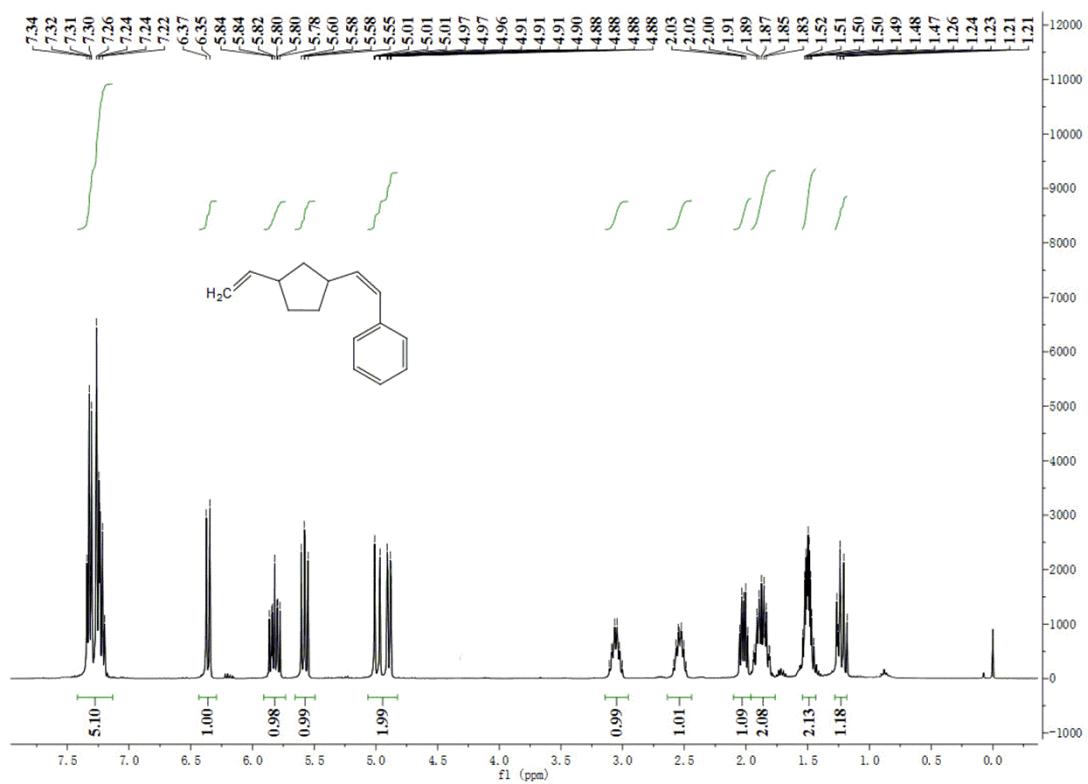
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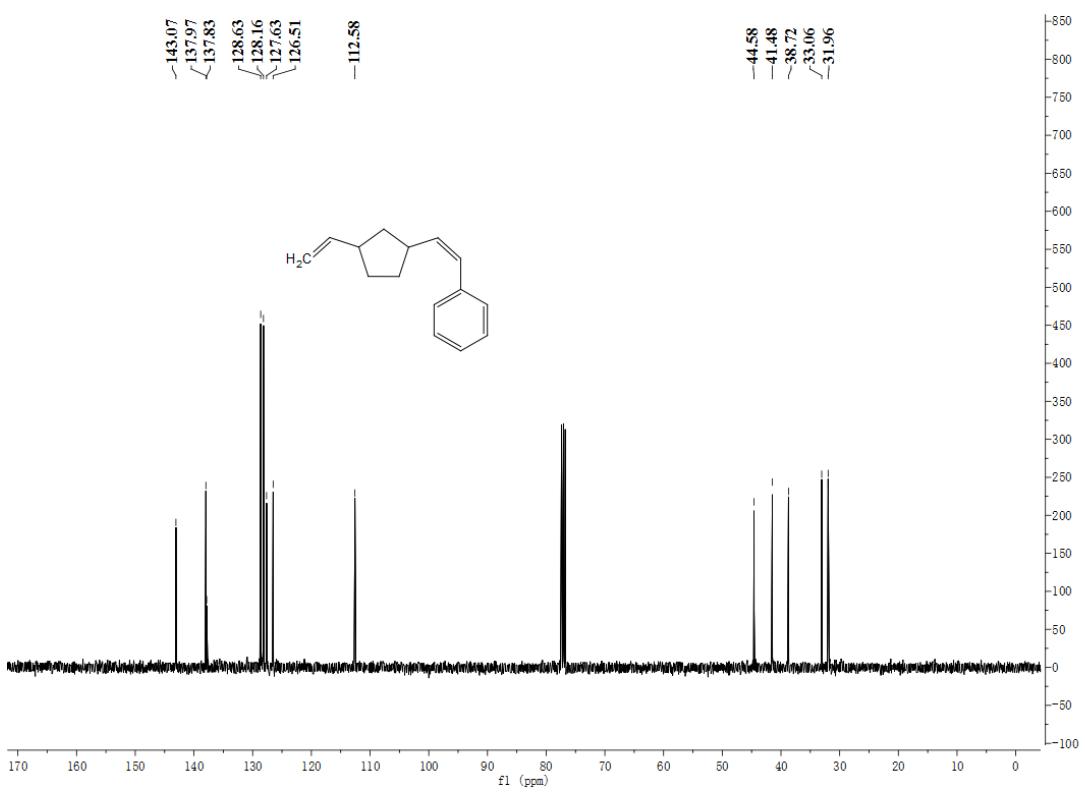
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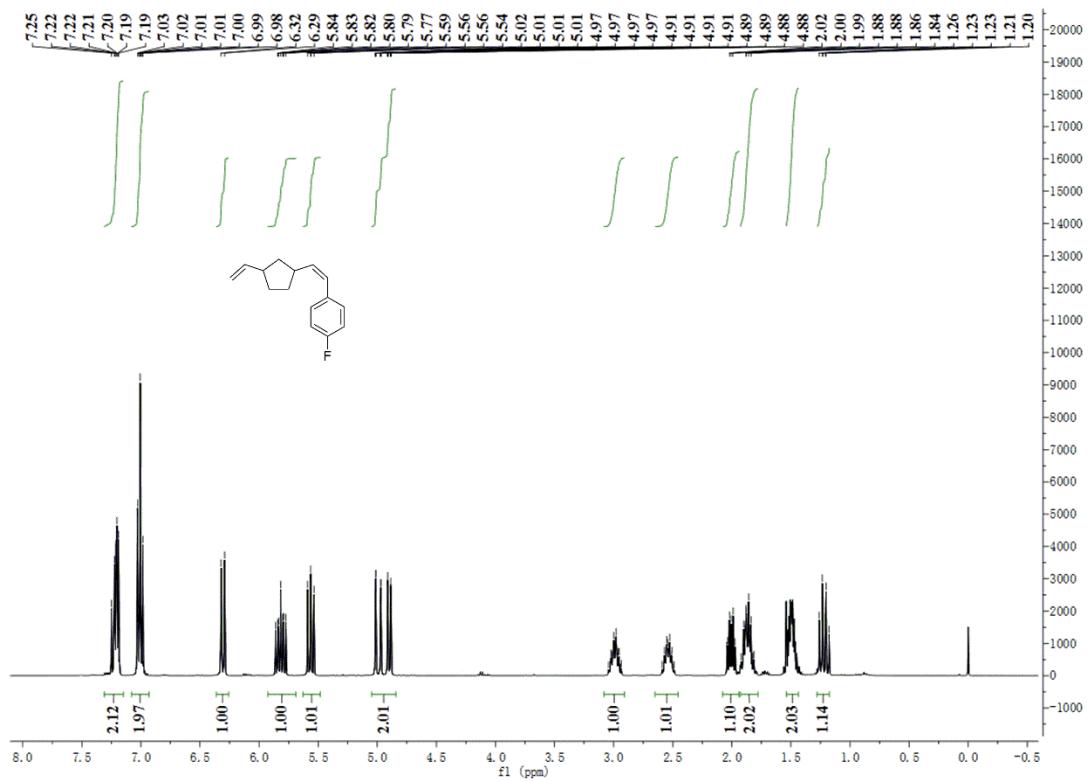
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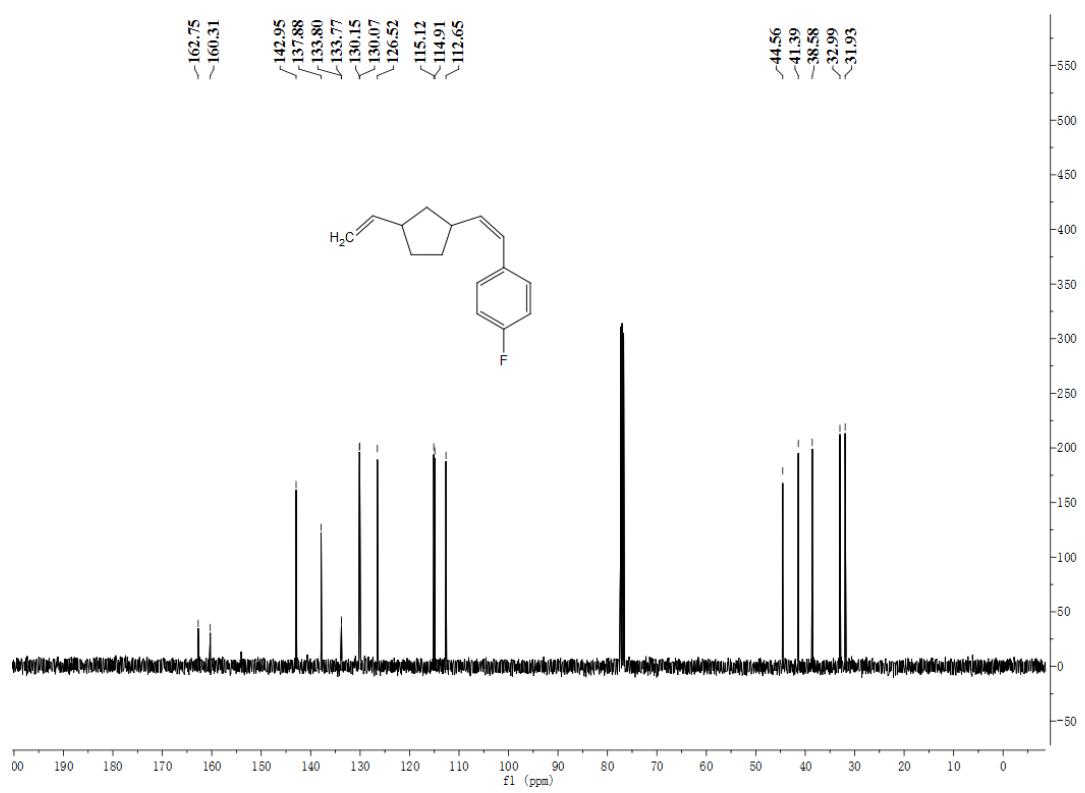
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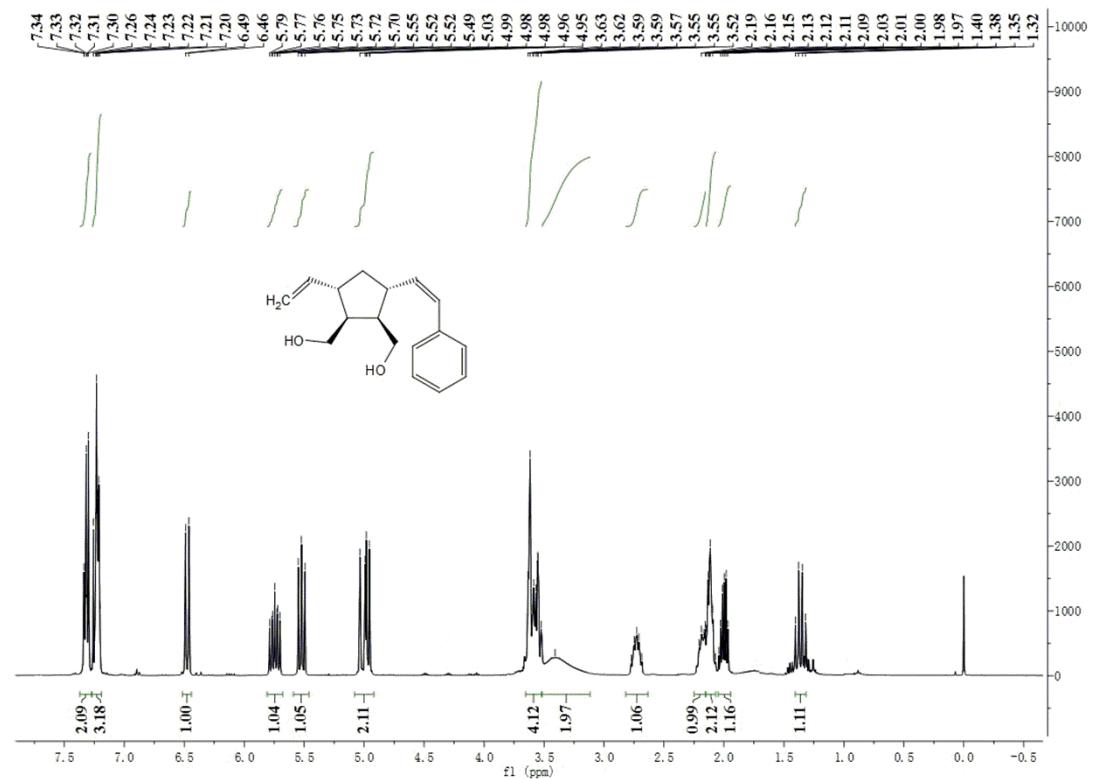
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S9
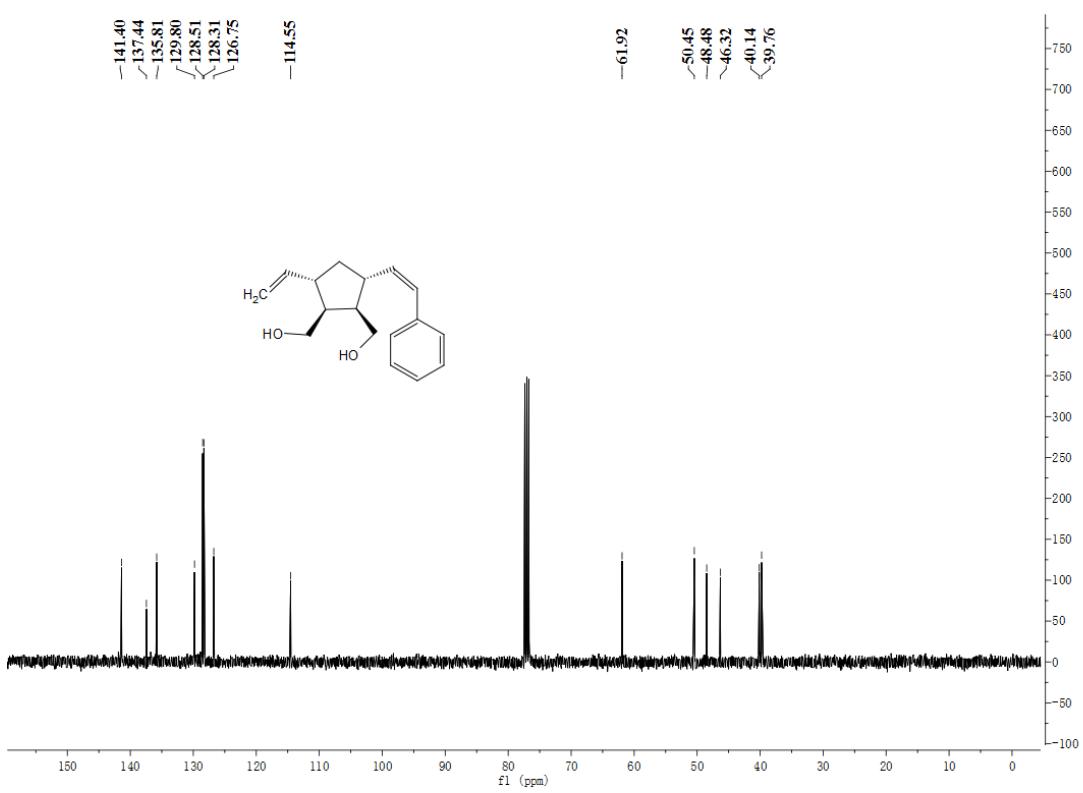
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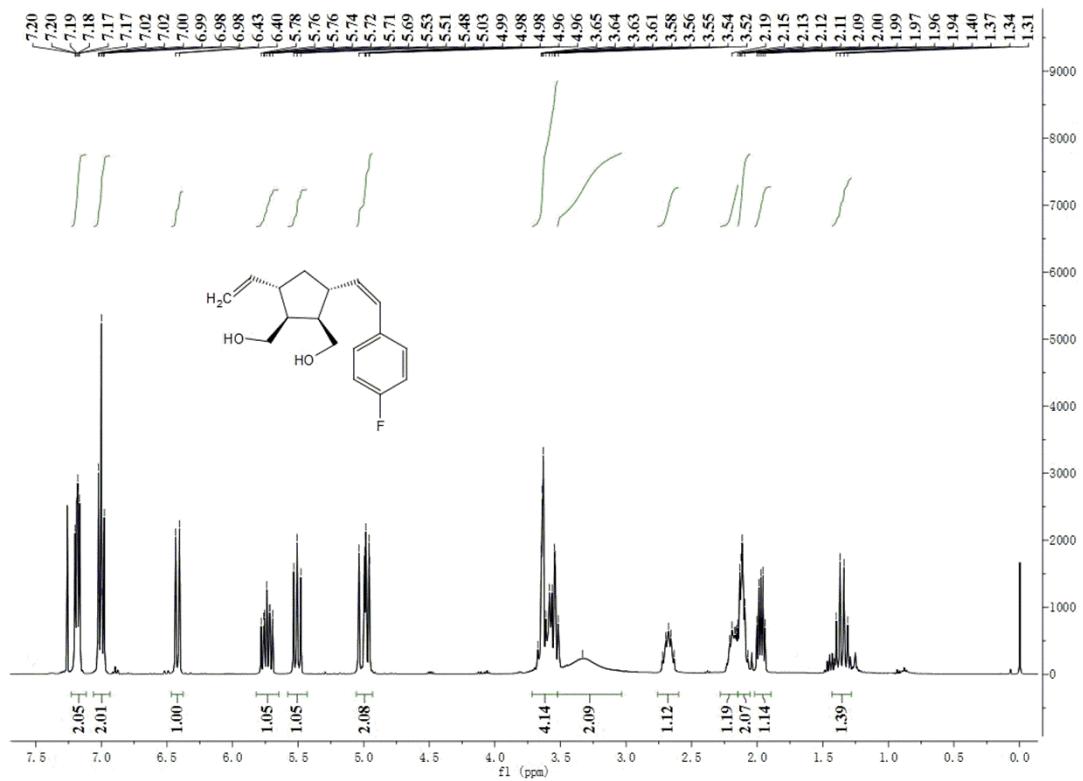
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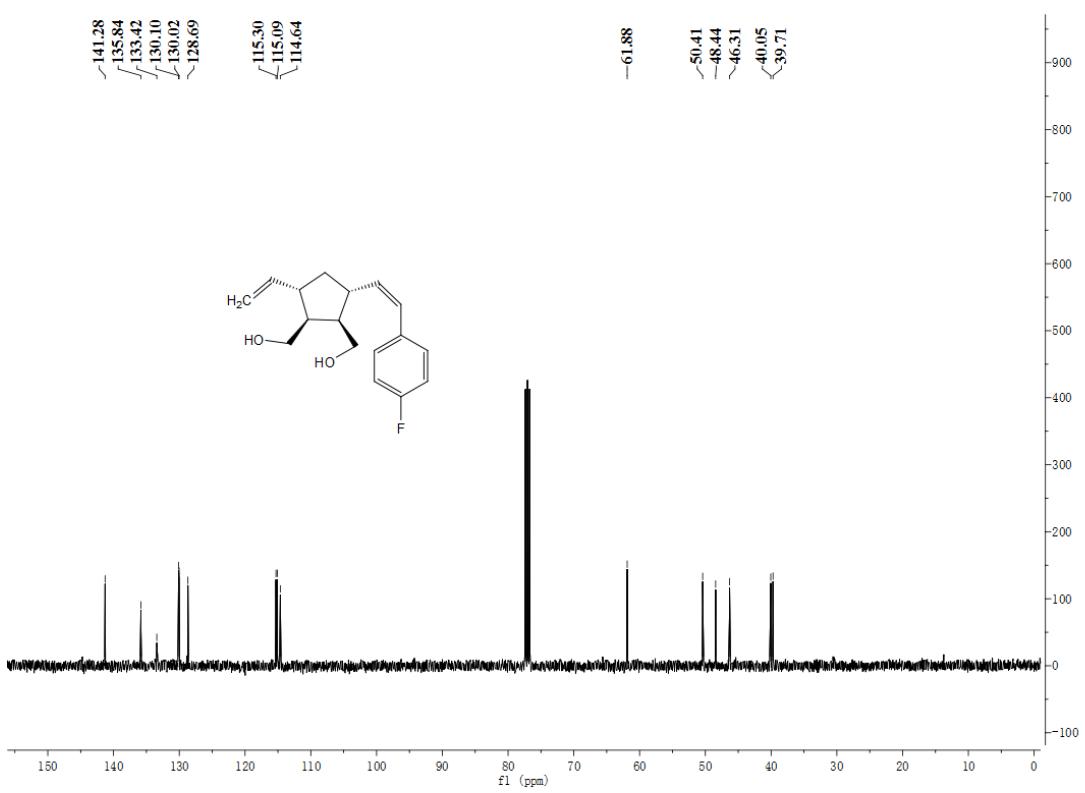
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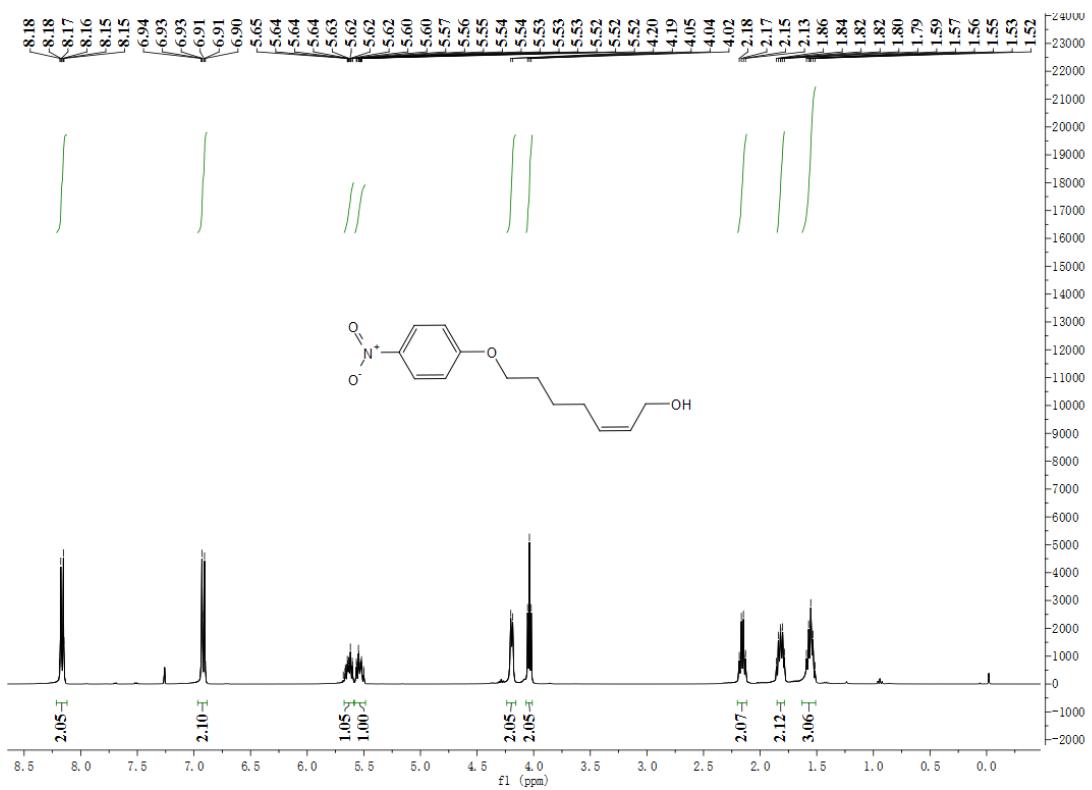
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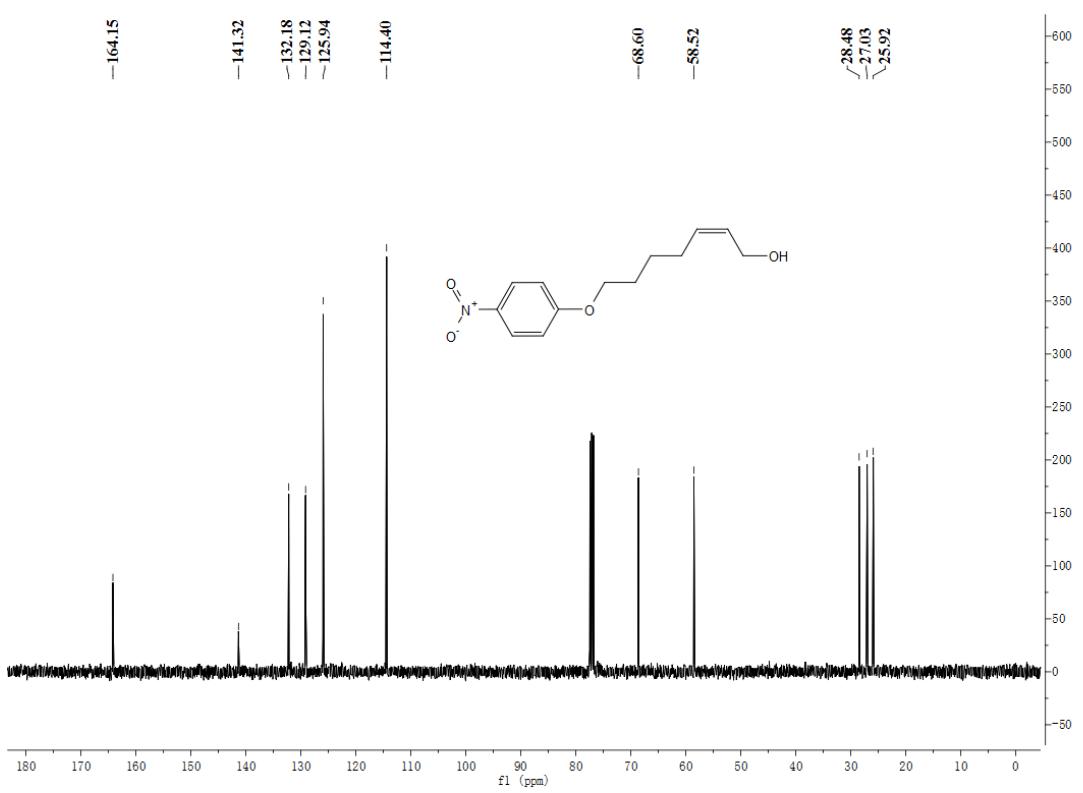
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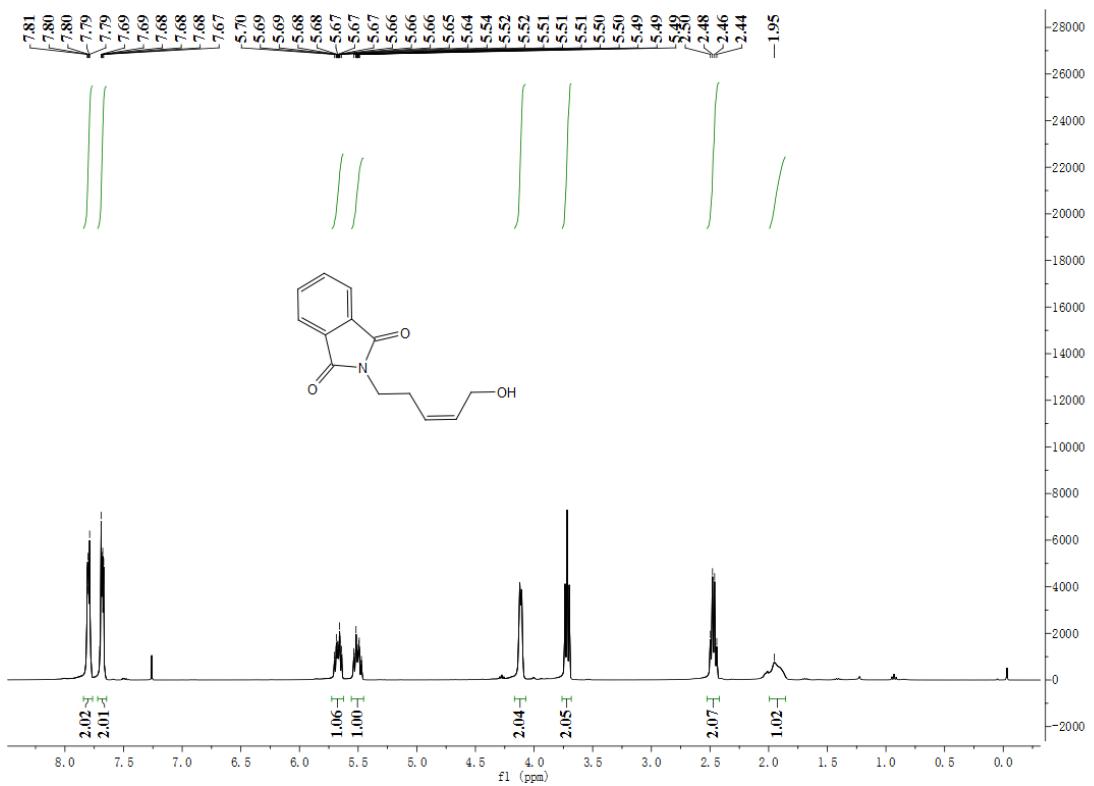
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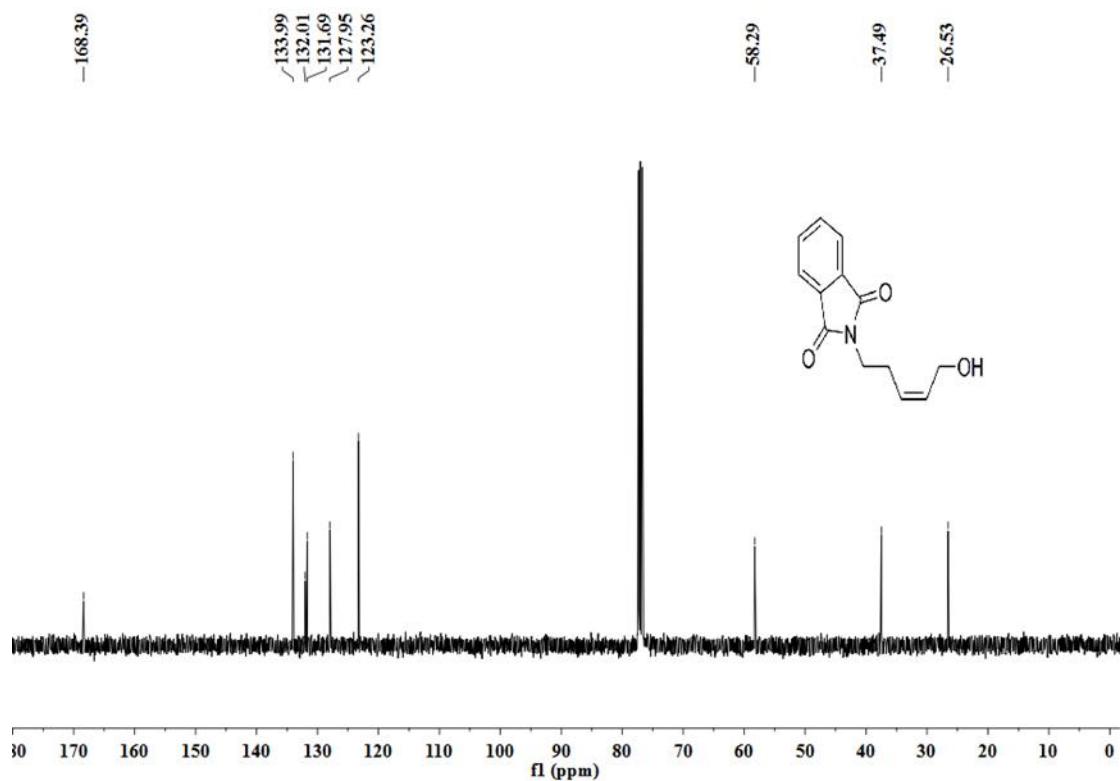
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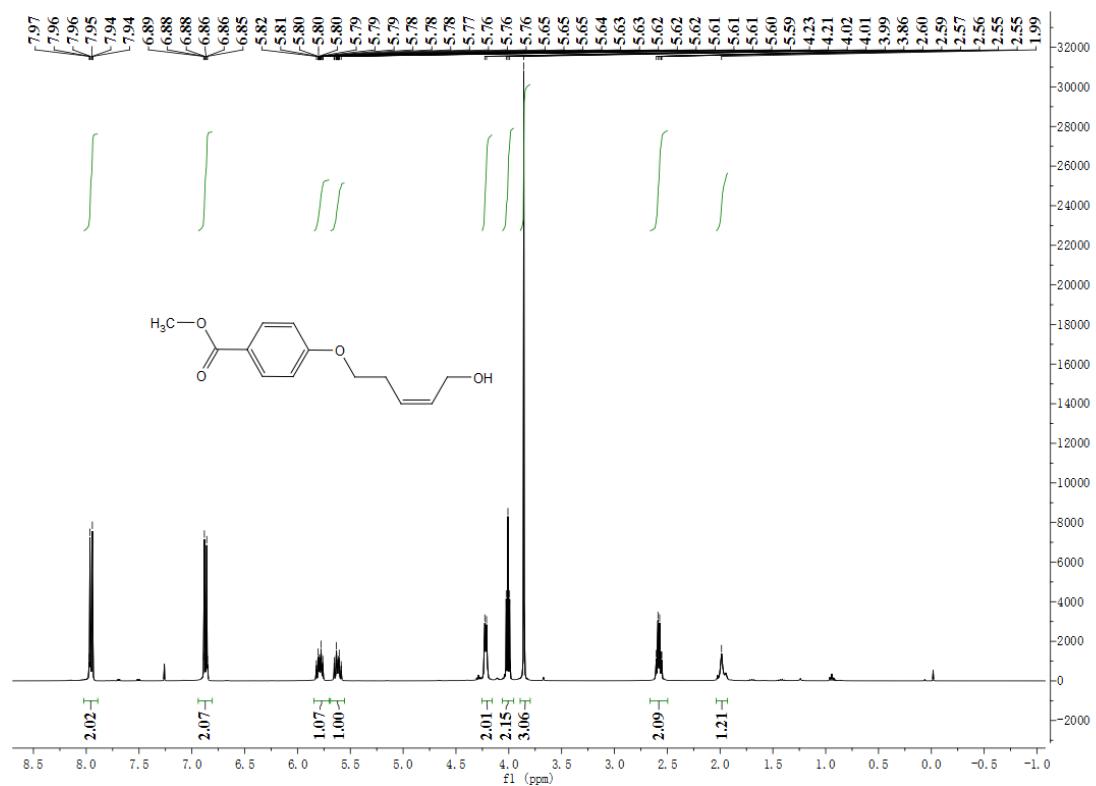
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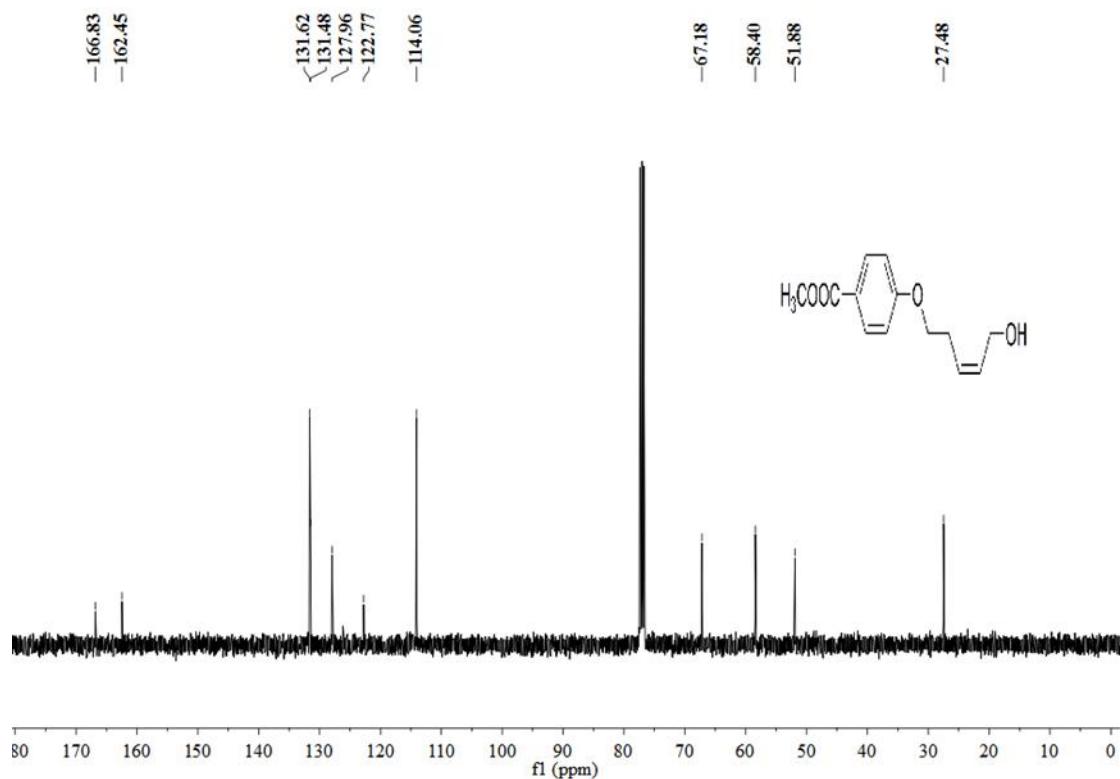
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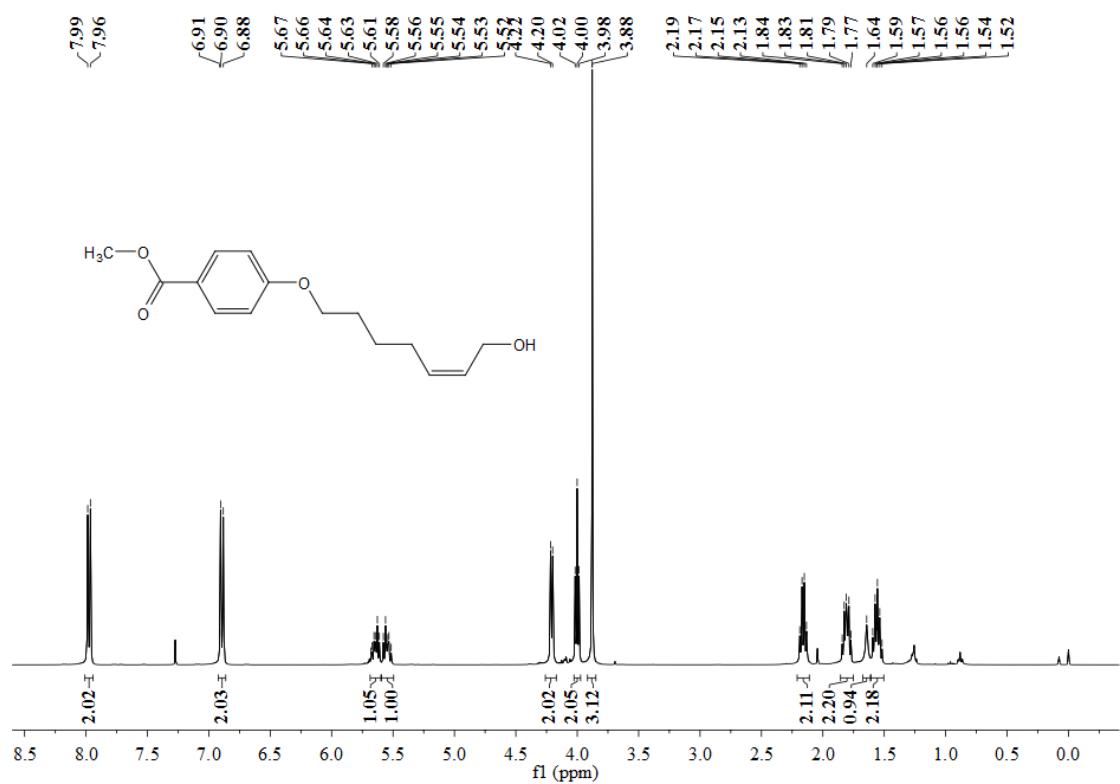
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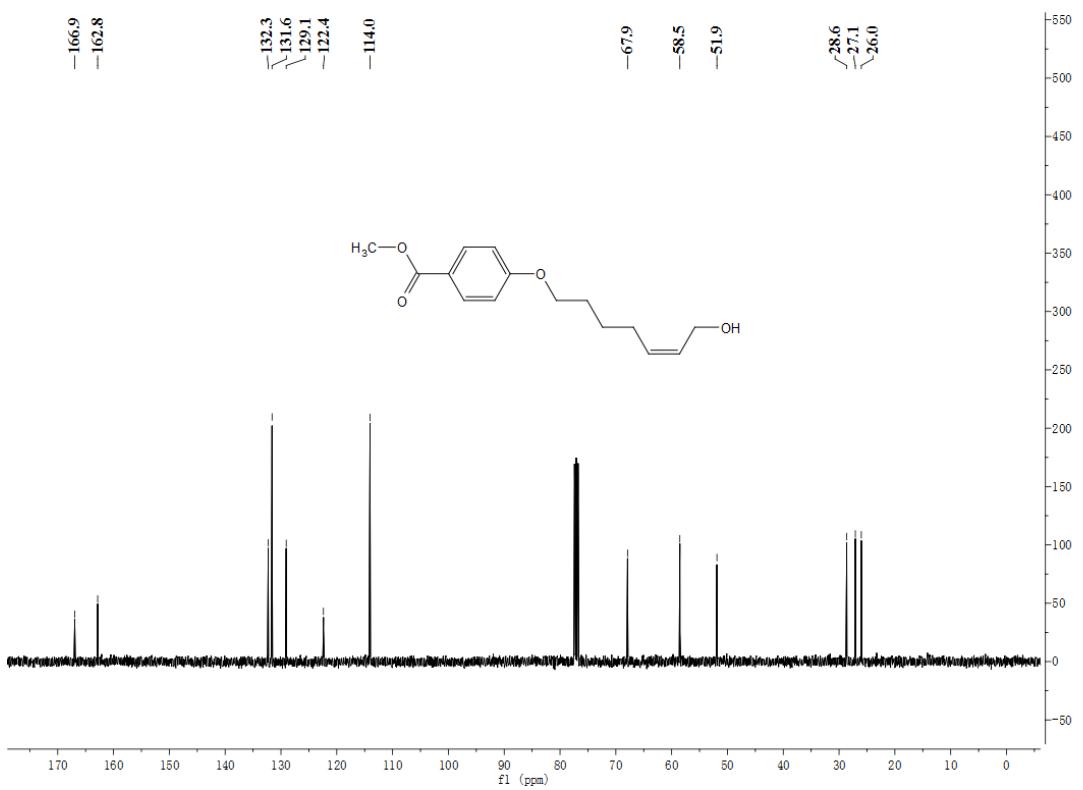
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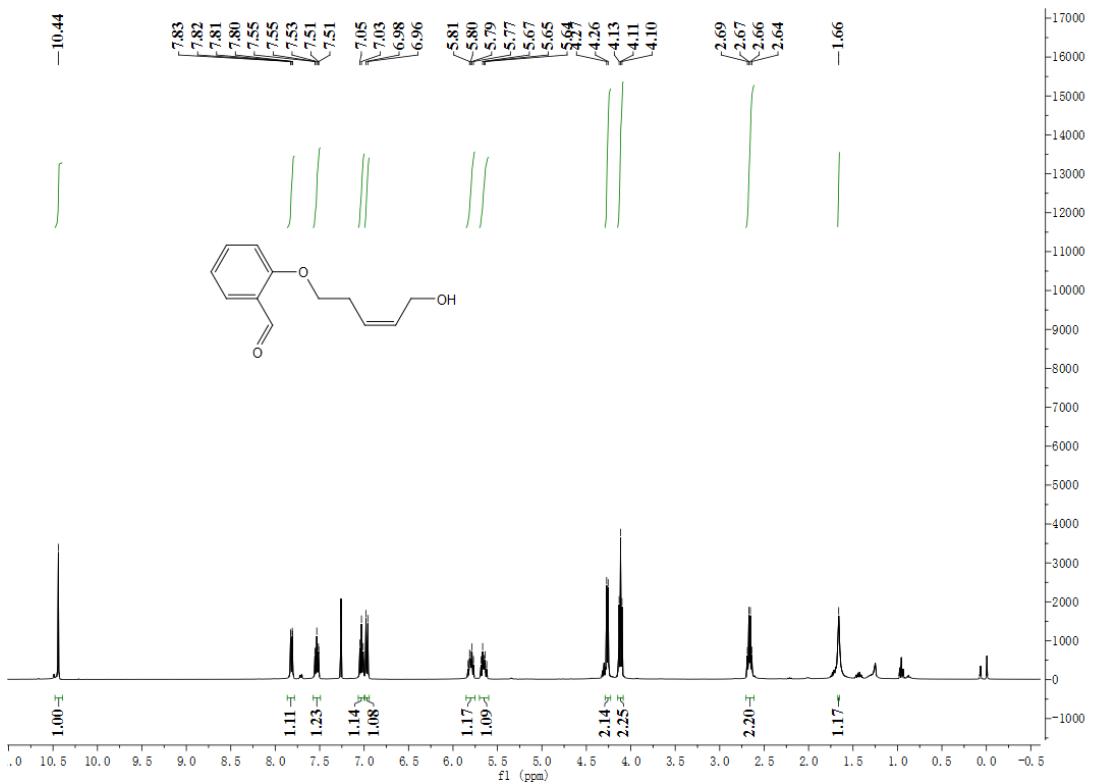
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S15
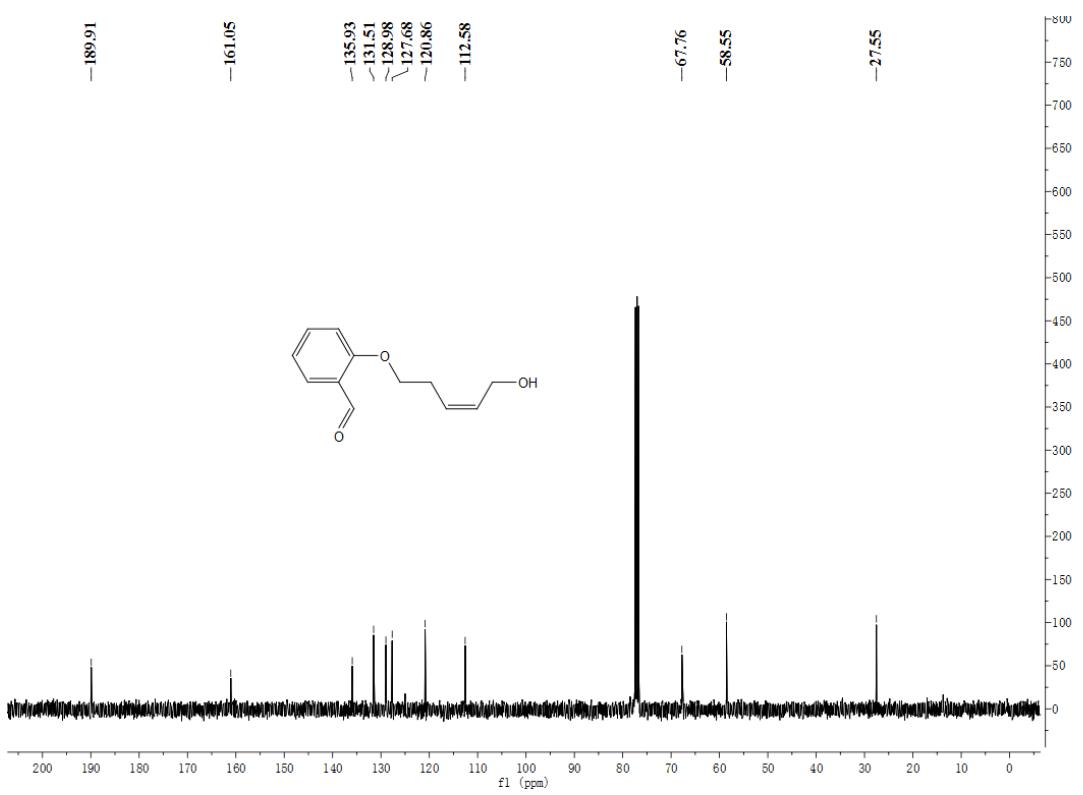
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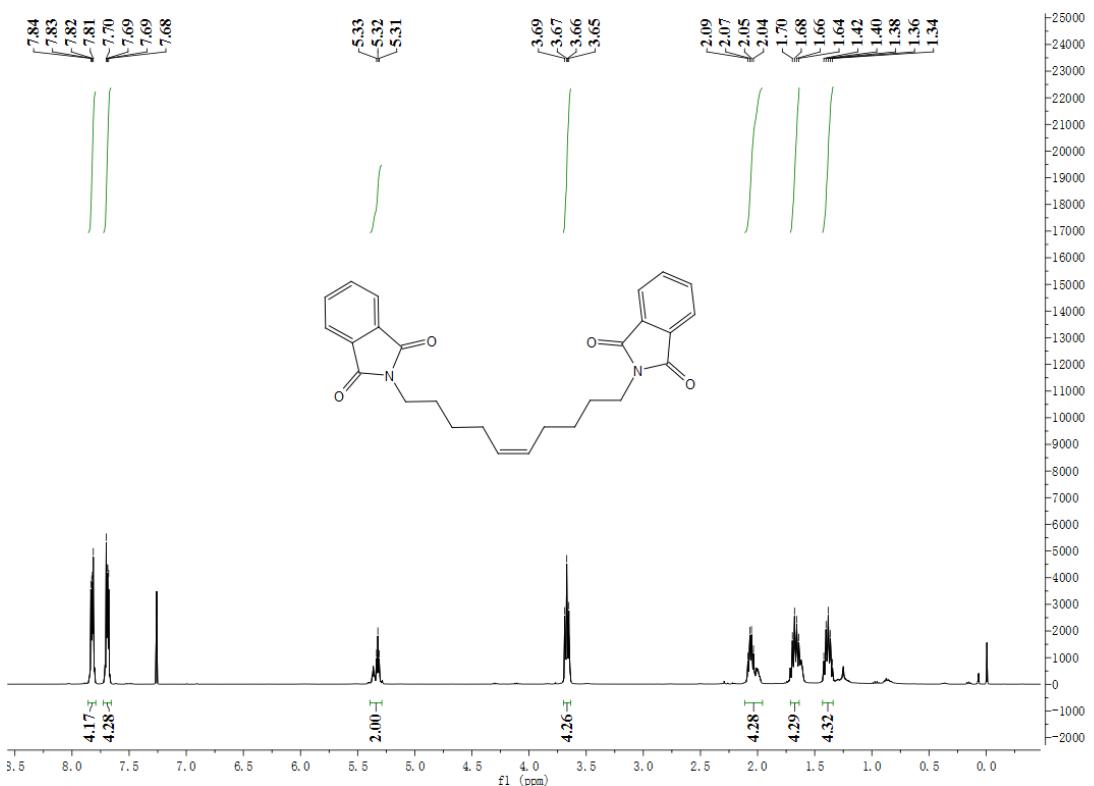
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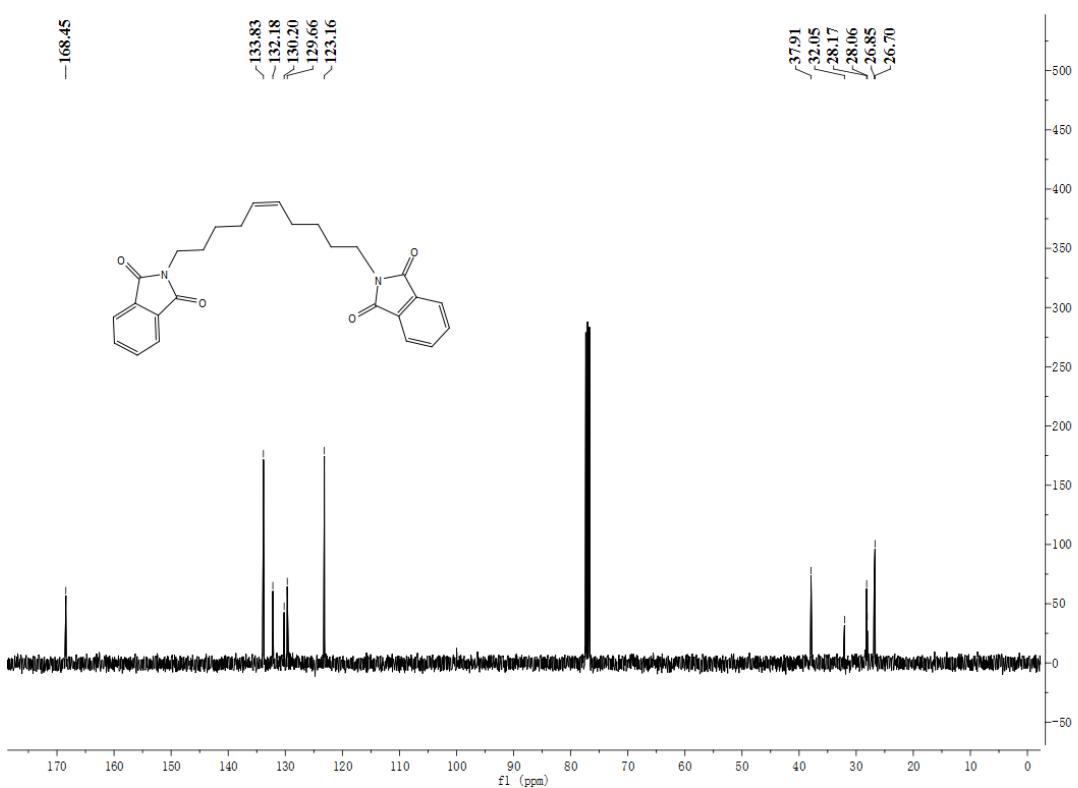
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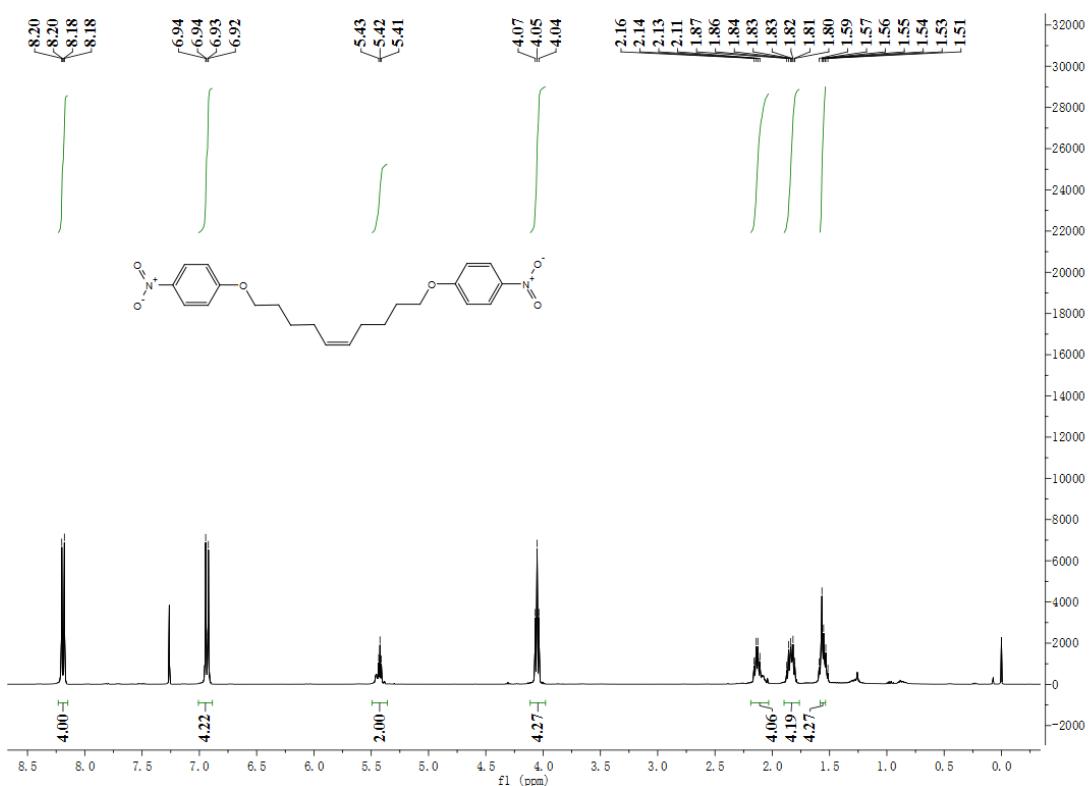
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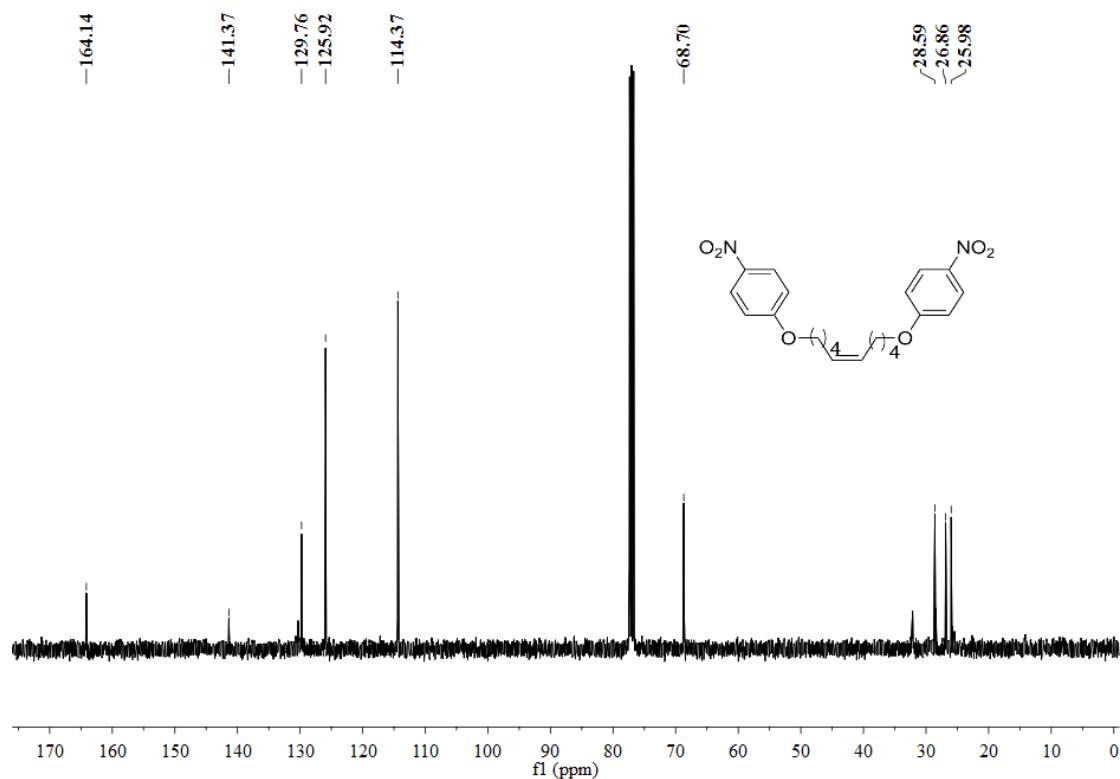
Figure S31. $^{13}C\{^1H\}$ NMR spectrum of **34** in $CDCl_3$ (100 Hz)
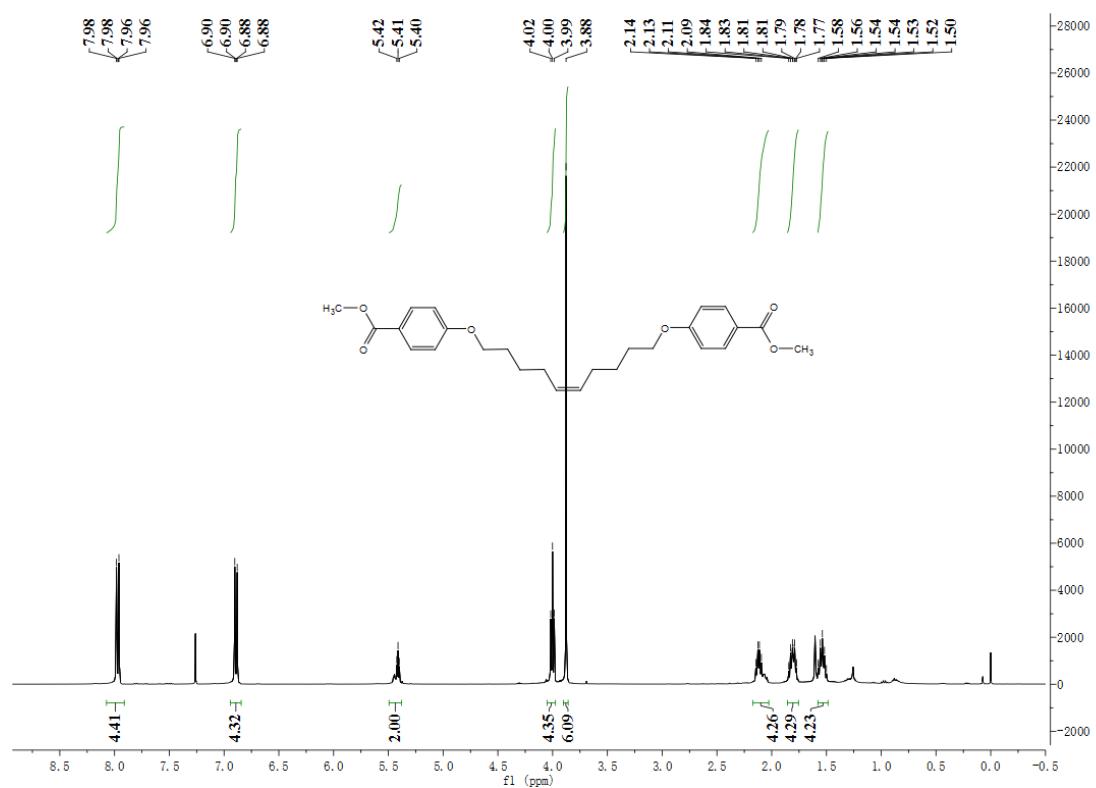
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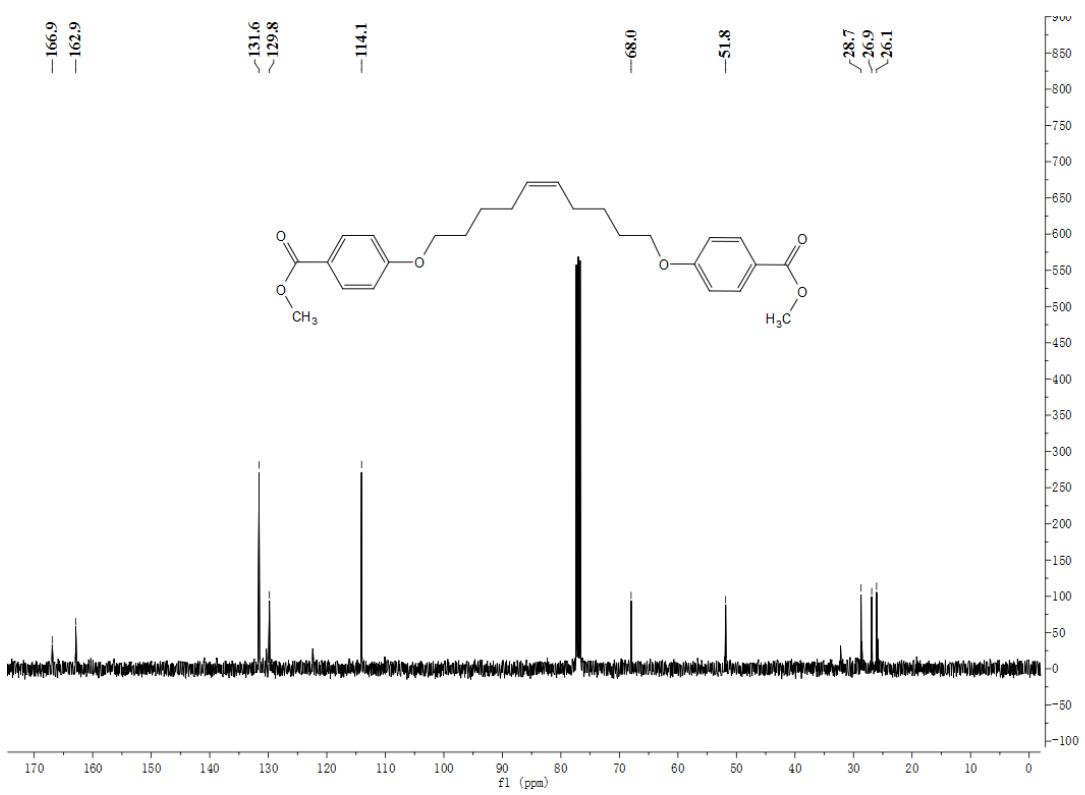
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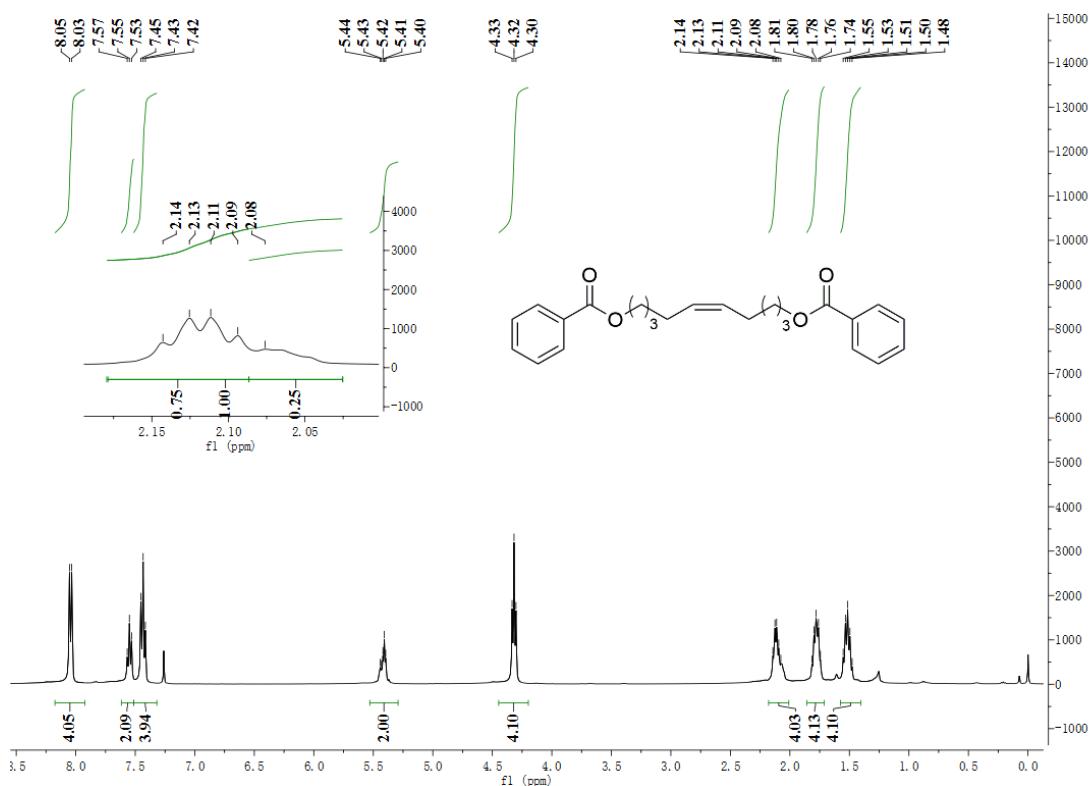
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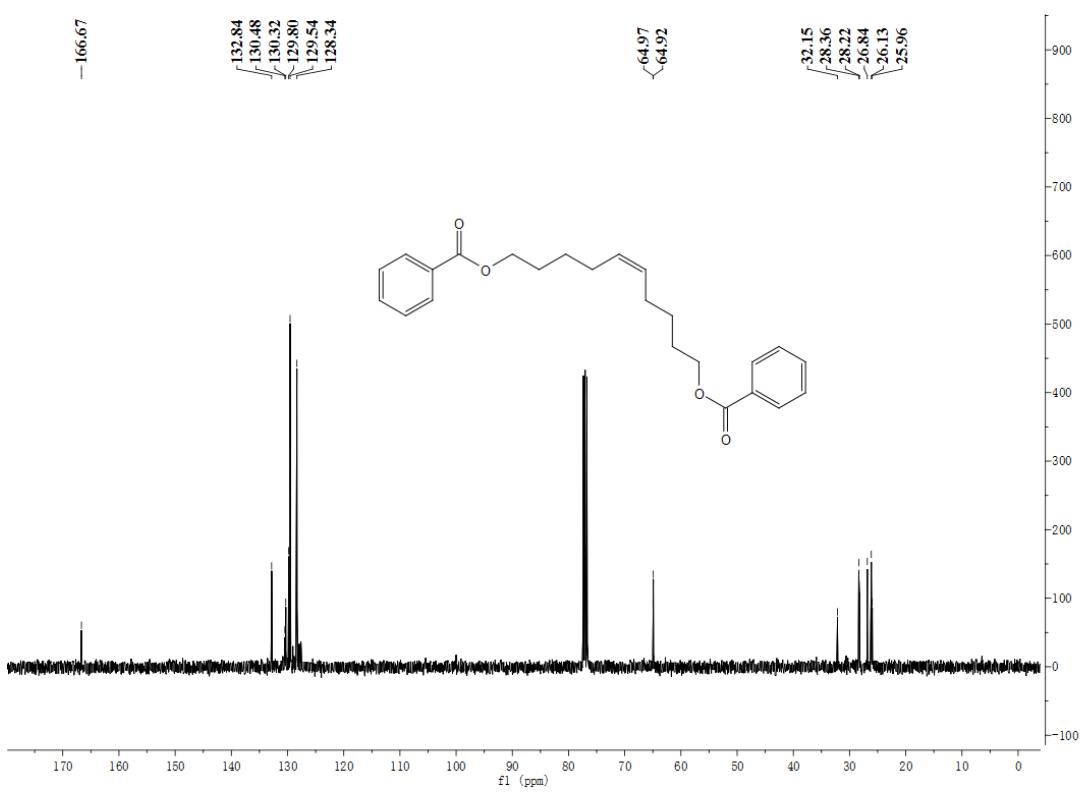
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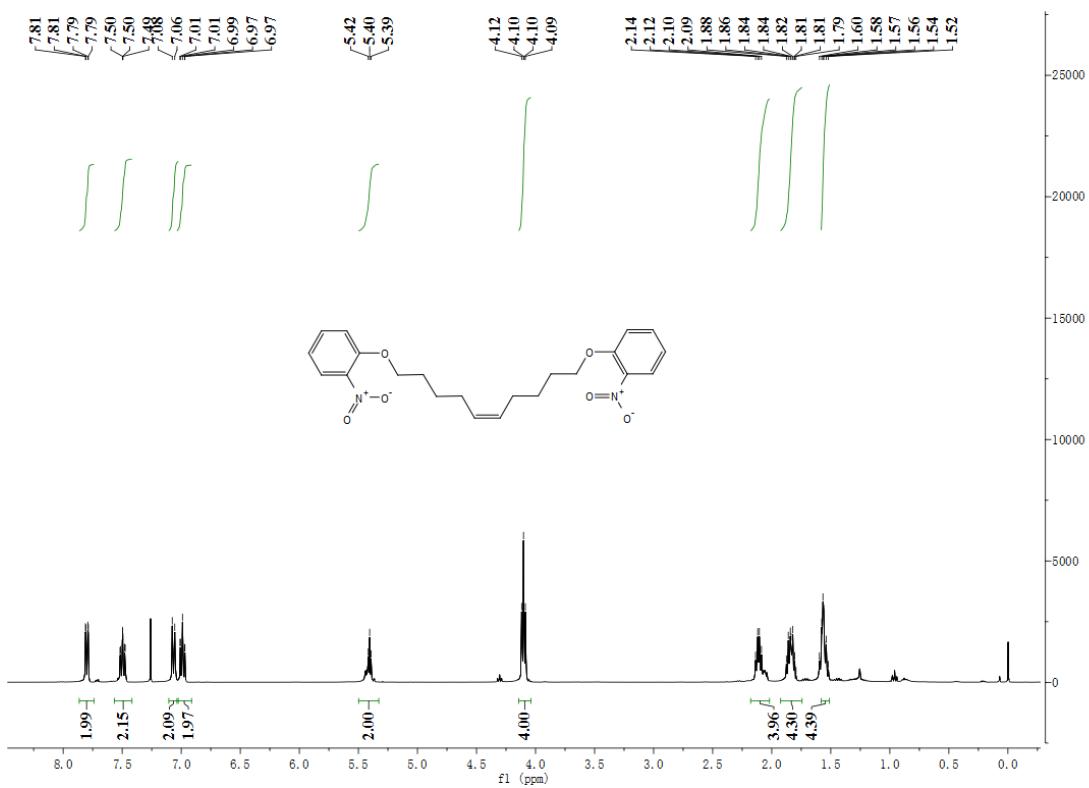
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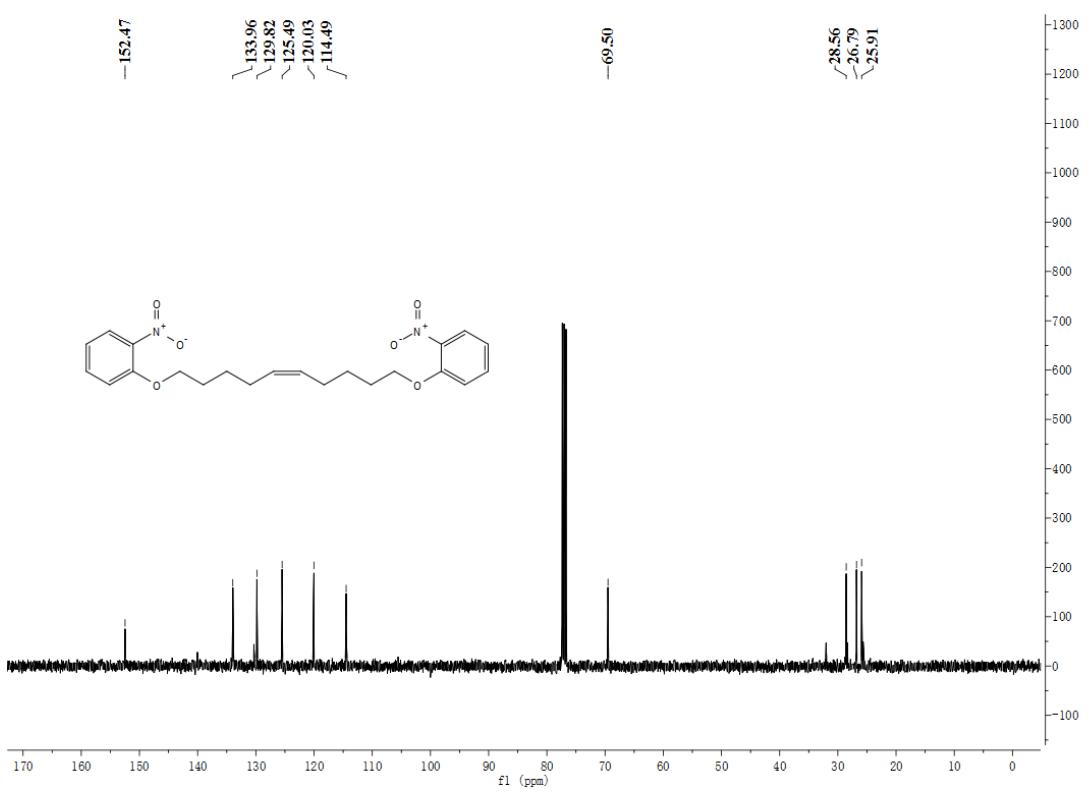
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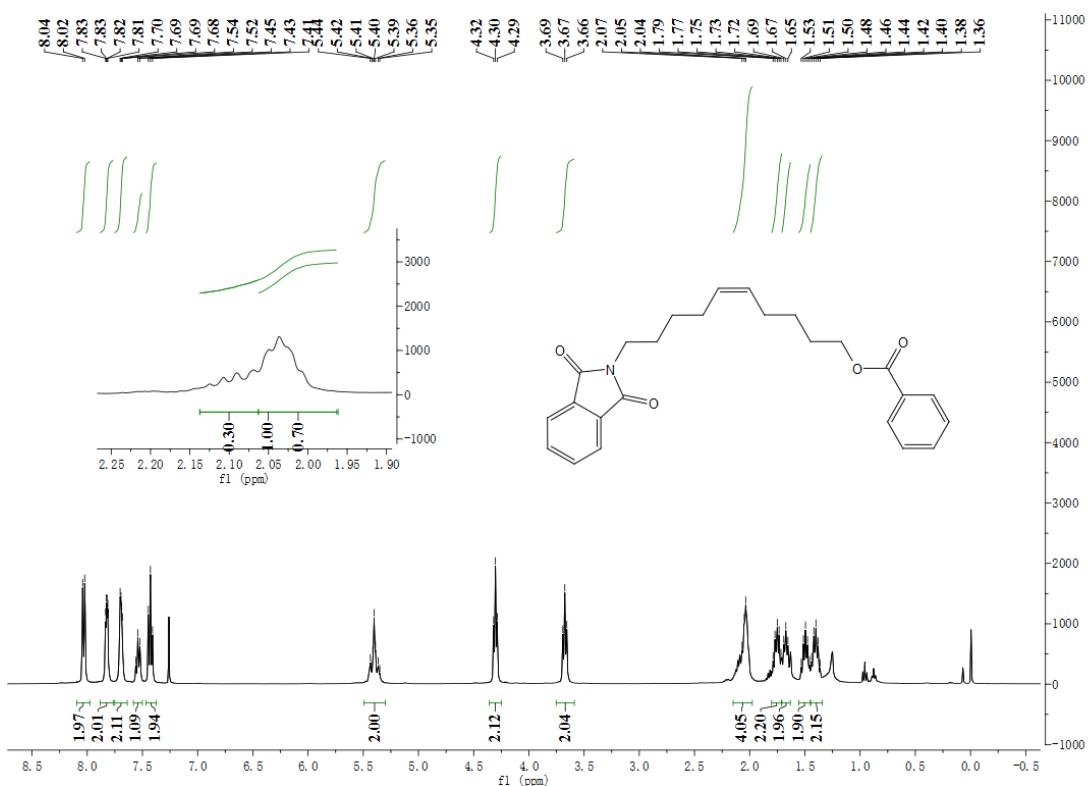
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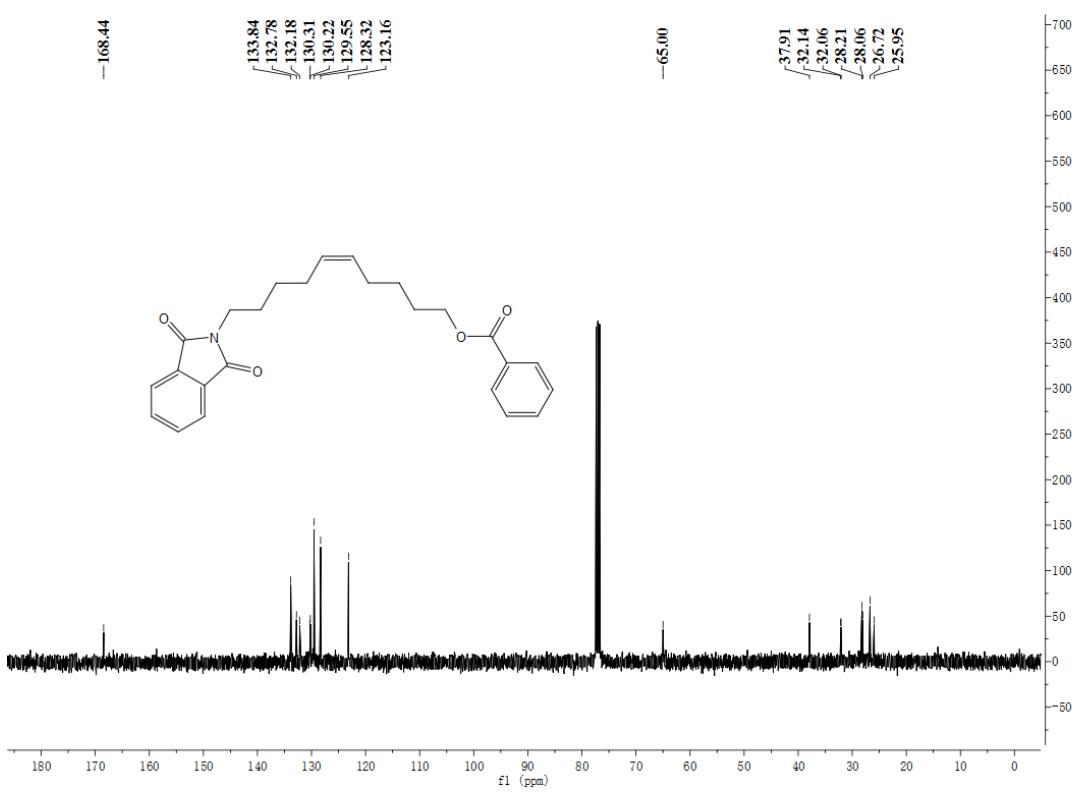
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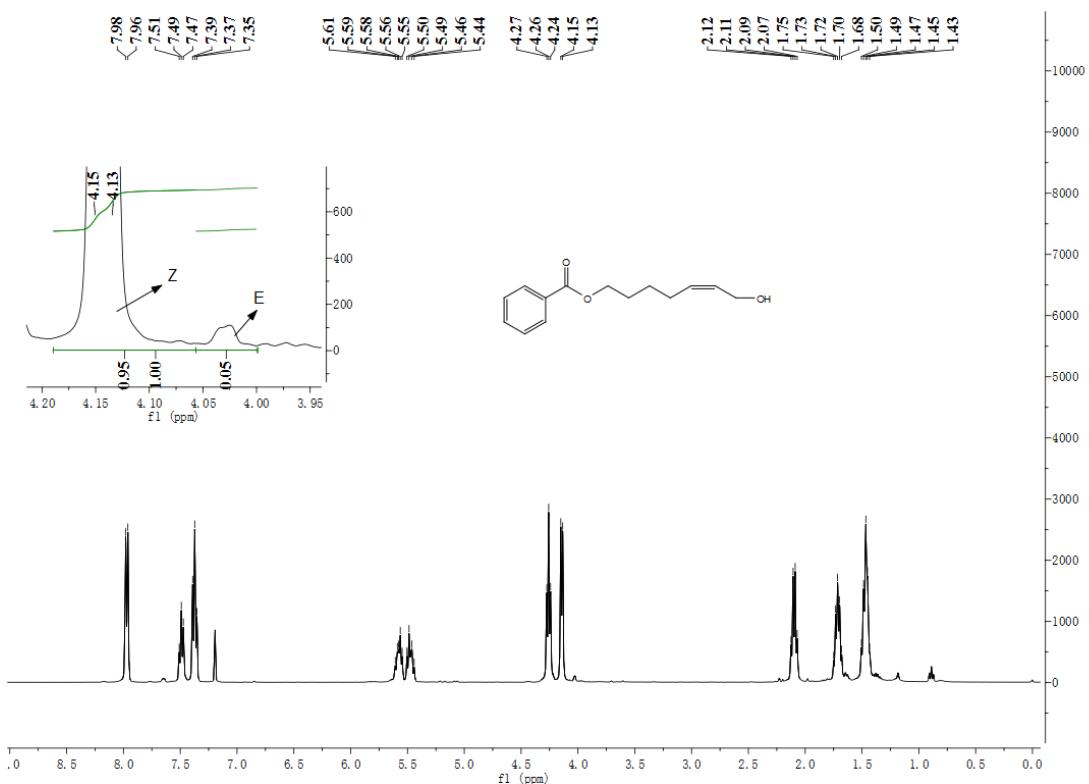
Figure S 40. ^1H NMR spectrum of **23** in CDCl$_3$ (400 Hz) (18th Days)
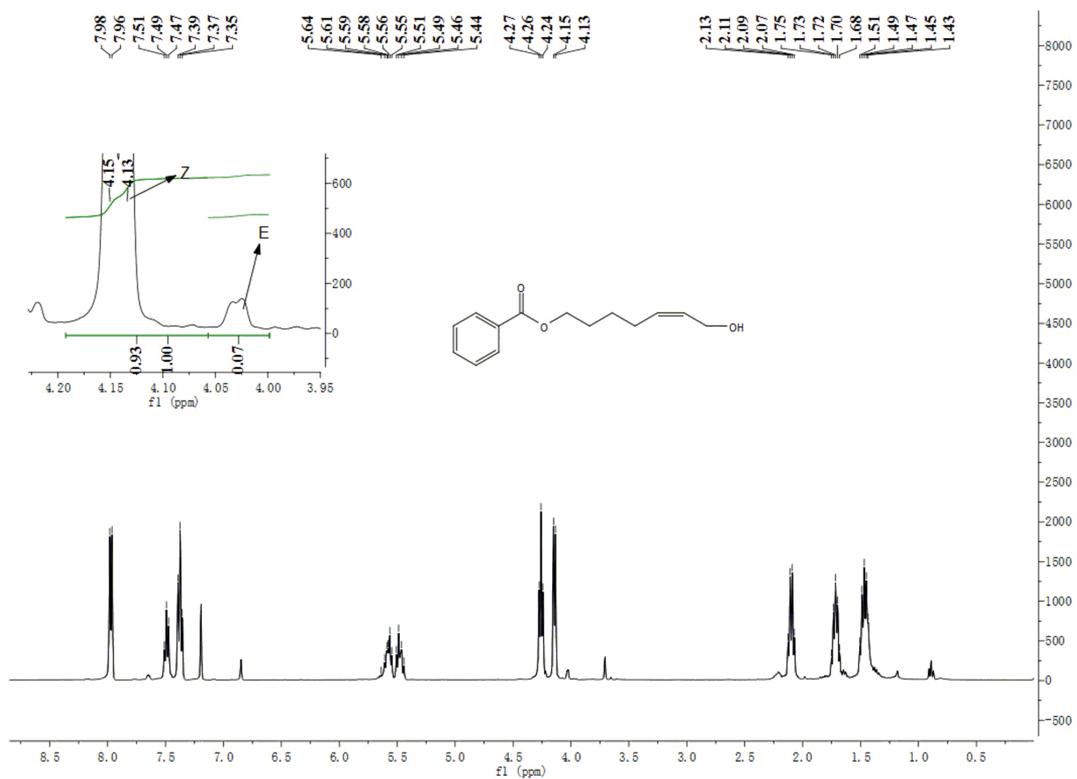
Figure S41. ^{1}H NMR spectrum of **23** in CDCl$_3$ (400 Hz) (28th Days)

Table S1. Crystal data and structure refinement for Ru-based complex

Identification Code	**B4**
Empirical formula	C$_{35}$H$_{39}$N$_2$O$_3$RuS$_2$
Formula weight	700.87
Temperature/K	135.00(10)
Crystal system	monoclinic
Space group	I2/a
a/Å	19.3991(4)
b/Å	11.4101(2)
c/Å	31.8762(7)
α/°	90
β/°	103.192(2)
γ/°	90
Volume/Å^3	6869.4(3)
Z	8
ρ$_{calc}$g/cm^3	1.355
μ/mm^{-1}	5.109
F(000)	2904.0
Crystal size/mm^3	0.25 × 0.2 × 0.18
Radiation	CuKα (λ = 1.54184)

2Θ range for data collection/°	8.256 to 134.152	
Index ranges	$-23 \leq h \leq 20$, $-9 \leq k \leq 13$, $-30 \leq l \leq 38$	
Reflections collected	12337	
Independent reflections	6122 [R_{int} = 0.0204, R_{sigma} = 0.0277]	
Data/restraints/parameters	6122/0/396	
Goodness-of-fit on F^2	1.037	
Final R indexes [I>=2σ (I)]	R_1 = 0.0280, wR_2 = 0.0705	
Final R indexes [all d ta]	R_1 = 0.0308, wR_2 = 0.0722	
Largest diff. peak/hole / e Å^{-3}	0.84/-0.72	

Table S2. Bond Lengths for Ru-based complex

Atom	Atom	Lenth/Å	Atom	Atom	Lenth/Å
Ru1	S1	2.3137(5)	C6	C9	1.499(3)
Ru1	S2	2.3785(5)	C10	C11	1.524(3)
Ru1	O1	2.2767(14)	C13	C14	1.395(3)
Ru1	C12	2.030(2)	C13	C18	1.401(3)
Ru1	C31	1.837(2)	C14	C15	1.398(4)
S1	C32	1.696(2)	C14	C19	1.507(4)
S2	C33	1.707(2)	C15	C16	1.378(4)
O1	C22	1.493(3)	C16	C17	1.389(4)
O1	C25	1.399(3)	C16	C20	1.514(4)
O2	C35	1.206(3)	C17	C18	1.391(4)
O3	C34	1.207(3)	C18	C21	1.510(4)
N1	C1	1.439(3)	C22	C23	1.516(3)
N1	C10	1.476(3)	C22	C24	1.514(3)
N1	C12	1.339(3)	C25	C26	1.397(3)
N2	C11	1.479(3)	C25	C30	1.387(3)
N2	C12	1.338(3)	C26	C27	1.394(3)
N2	C13	1.435(3)	C26	C31	1.447(3)
C1	C2	1.393(3)	C27	C28	1.380(4)
C1	C6	1.409(3)	C28	C29	1.388(4)
C2	C3	1.400(3)	C29	C30	1.381(4)
C2	C7	1.504(3)	C32	C33	1.382(3)
C3	C4	1.385(3)	C32	C35	1.480(3)
C4	C5	1.392(3)	C33	C34	1.473(3)
C4	C8	1.510(3)	C34	C35	1.553(3)
C5	C6	1.388(3)			

Table S3. Bond Angles for Ru-based complex

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
S1	Ru1	S2	90.635(19)	C14	C13	N2	120.0(2)
O1	Ru1	S1	170.49(4)	C14	C13	C18	121.6(2)
O1	Ru1	S2	90.68(4)	C18	C13	N2	118.3(2)
C12	Ru1	S1	85.60(6)	C13	C14	C15	117.8(2)
C12	Ru1	S2	143.96(6)	C13	C14	C19	121.9(2)
C12	Ru1	O1	98.80(7)	C15	C14	C19	120.2(2)
C31	Ru1	S1	91.17(7)	C16	C15	C14	122.0(3)
C31	Ru1	S2	117.04(7)	C15	C16	C17	118.8(2)
C31	Ru1	O1	79.85(8)	C15	C16	C20	120.8(3)
C31	Ru1	C12	98.89(9)	C17	C16	C20	120.4(3)
C32	S1	Ru1	100.54(8)	C16	C17	C18	121.6(3)
C33	S2	Ru1	98.69(8)	C13	C18	C21	121.5(2)
C22	O1	Ru1	119.92(13)	C17	C18	C13	118.1(2)
C25	O1	Ru1	108.45(12)	C17	C18	C21	120.5(2)
C25	O1	C22	118.38(16)	O1	C22	C23	110.86(19)
C1	N1	C10	122.61(17)	O1	C22	C24	113.0(2)
C12	N1	C1	123.45(17)	C24	C22	C23	113.50(19)
C12	N1	C10	112.93(17)	C26	C25	O1	114.21(19)
C12	N2	C11	112.58(17)	C30	C25	O1	124.1(2)
C12	N2	C13	126.34(18)	C30	C25	C26	121.6(2)
C13	N2	C11	120.45(17)	C25	C26	C31	118.5(2)
C2	C1	N1	120.59(18)	C27	C26	C25	118.8(2)
C2	C1	C6	121.28(19)	C27	C26	C31	122.6(2)
C6	C1	N1	118.07(19)	C28	C27	C26	119.9(3)
C1	C2	C3	118.3(2)	C27	C28	C29	120.2(3)
C1	C2	C7	122.7(2)	C30	C29	C28	121.1(3)
C3	C2	C7	118.9(2)	C29	C30	C25	118.3(3)
C4	C3	C2	121.7(2)	C26	C31	Ru1	118.89(16)
C3	C4	C5	118.5(2)	C33	C32	S1	125.05(18)
C3	C4	C8	121.1(2)	C33	C32	C35	93.24(19)
C5	C4	C8	120.4(2)	C35	C32	S1	141.70(18)
C6	C5	C4	122.0(2)	C32	C33	S2	125.06(18)
C1	C6	C9	121.18(19)	C32	C33	C34	93.39(19)

A	B	C				
C5	C6	C1		118.1(2)	C34	C33	S2		141.55(18)
C5	C6	C9		120.7(2)	O3	C34	C33		137.4(2)
N1	C10	C11		102.62(17)	O3	C34	C35		135.7(2)
N2	C11	C10		102.96(17)	O3	C34	C35		135.7(2)
N1	C12	Ru1		115.90(15)	C33	C34	C35		86.91(18)
N2	C12	Ru1		134.13(15)	O2	C35	C32		137.4(2)
N2	C12	N1		108.90(18)	O2	C35	C34		136.2(2)
					C32	C35	C34	86.46(18)	

Table S4. Torsion Angles for Ru-based complex.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ru1	S1	C32	C33	-1.4(2)	C10	N1	C12	N2	0.7(2)
Ru1	S1	C32	C35	178.0(3)	C11	N2	C12	Ru1	-168.11(17)
Ru1	S2	C33	C32	0.3(2)	C11	N2	C12	N1	-0.9(3)
Ru1	S2	C33	C34	-178.7(3)	C11	N2	C13	C14	85.0(3)
Ru1	O1	C22	C23	-90.44(19)	C11	N2	C13	C18	-92.2(3)
Ru1	O1	C22	C24	140.87(16)	C12	Ru1	C31	C26	-96.12(18)
Ru1	O1	C25	C26	2.2(2)	C12	N1	C1	C2	97.2(2)
Ru1	O1	C25	C30	-174.0(2)	C12	N1	C1	C6	-85.4(3)
S1	Ru1	C31	C26	178.15(17)	C12	N1	C10	C11	-0.3(2)
S1	C32	C33	S2	0.9(3)	C12	N2	C11	C10	0.7(3)
S1	C32	C33	C34	-179.78(17)	C12	N2	C13	C14	-104.8(3)
S1	C32	C35	O2	-0.6(5)	C12	N2	C13	C18	78.0(3)
S1	C32	C35	C34	179.9(2)	C13	N2	C11	C10	172.13(19)
S2	Ru1	C31	C26	86.84(18)	C13	N2	C12	Ru1	21.0(3)
S2	C33	C34	O3	-1.8(5)	C13	N2	C12	N1	-171.7(2)
S2	C33	C34	C35	178.6(2)	C13	C14	C15	C16	2.4(4)
O1	Ru1	C31	C26	1.30(17)	C14	C13	C18	C17	1.2(3)
O1	C25	C26	C27	-178.2(2)	C14	C13	C18	C21	-178.9(2)
O1	C25	C26	C31	-1.5(3)	C14	C15	C16	C17	-0.5(4)
O1	C25	C30	C29	177.2(3)	C14	C15	C16	C20	179.1(3)
O3	C34	C35	O2	1.4(5)	C15	C16	C17	C18	-1.1(4)
O3	C34	C35	C32	-179.1(3)	C16	C17	C18	C13	0.7(4)
N1	C1	C2	C3	179.68(19)	C16	C17	C18	C21	-179.2(2)
N1	C1	C2	C7	1.8(3)	C18	C13	C14	C15	-2.7(3)
N1	C1	C6	C5	-179.18(18)	C18	C13	C14	C19	174.5(2)
N1	C1	C6	C9	-0.3(3)	C19	C14	C15	C16	-174.9(2)
N1	C10	C11	N2	-0.2(2)	C20	C16	C17	C18	179.3(3)
N2	C13	C14	C15	-179.8(2)	C22	O1	C25	C26	-138.8(2)
N2	C13	C14	C19	-2.6(3)	C22	O1	C25	C30	44.9(3)

N2	C13	C18	C17	178.3(2)	C25	O1	C22	C23	46.1(3)
N2	C13	C18	C21	-1.8(3)	C25	O1	C22	C24	-82.6(2)
C1	N1	C10	C11	-169.15(19)	C25	C26	C27	C28	1.1(4)
C1	N1	C12	Ru1	-20.7(3)	C25	C26	C31	Ru1	-0.4(3)
C1	N1	C12	N2	169.47(19)	C26	C25	C30	C29	1.2(4)
C1	C2	C3	C4	-1.5(3)	C26	C27	C28	C29	0.1(5)
C2	C1	C6	C5	-1.8(3)	C27	C26	C31	Ru1	176.2(2)
C2	C1	C6	C9	177.05(19)	C27	C28	C29	C30	-0.7(6)
C2	C3	C4	C5	0.2(3)	C28	C29	C30	C25	0.1(5)
C2	C3	C4	C8	-179.0(2)	C30	C25	C26	C27	-1.8(4)
C3	C4	C5	C6	0.4(3)	C30	C25	C26	C31	174.9(2)
C4	C5	C6	C1	0.4(3)	C31	C26	C27	C28	-175.5(3)
C4	C5	C6	C9	-178.5(2)	C32	C33	C34	O3	179.0(3)
C6	C1	C2	C3	2.4(3)	C32	C33	C34	C35	-0.52(18)
C6	C1	C2	C7	-175.5(2)	C33	C32	C35	O2	179.0(3)
C7	C2	C3	C4	176.4(2)	C33	C32	C35	C34	-0.52(18)
C8	C4	C5	C6	179.6(2)	C33	C34	C35	O2	-179.0(3)
C10	N1	C1	C2	-95.1(3)	C33	C34	C35	C32	0.49(17)
C10	N1	C1	C6	82.3(2)	C35	C32	C33	S2	-178.80(17)
C10	N1	C12	Ru1	170.57(14)	C35	C32	C33	C34	0.55(19)

The data of DFT calculations

Cat._L1

E(BP86)= -2433.65493267 Hartree

Ru	-0.18236200	-0.40239900	0.37089700
S	-1.20921000	0.94892400	1.98449700
S	-1.90929500	-2.06043300	0.56350500
O	1.00620700	-1.86901100	-0.94816200
O	-4.74289000	1.21826200	3.11135200
O	-5.42732800	-1.76442900	1.72278000
N	-0.74203800	1.85530900	-1.36680300
N	1.40466500	1.94604500	-0.86390700
C	-1.99271900	1.17000500	-1.56967400
C	-3.13273100	1.54843200	-0.82382700
C	-4.27298200	0.73210200	-0.91489400
C	-4.31231700	-0.40998900	-1.73448800
C	-3.19762100	-0.68533600	-2.54850100
C	-2.03125800	0.09038600	-2.48755100
C	-3.16109800	2.80160100	0.01782600
C	-5.51555700	-1.32231100	-1.71455800
C	-0.84999100	-0.21325100	-3.38207400
C	-0.25269200	2.97101800	-2.20153600
C	1.17555200	3.18276500	-1.64933800
C	0.26116800	1.23892600	-0.67739500
C	2.68656500	1.62640100	-0.31506100
C	3.02996000	2.07961300	0.97507000
C	4.29996000	1.73600500	1.47404200
C	5.21133700	0.97398500	0.72348700
C	4.83234700	0.54630000	-0.56296500
C	3.57578900	0.85799000	-1.09972700
C	2.05331100	2.88095700	1.80100900
C	6.56237800	0.59461000	1.28454500
C	3.16426900	0.35793900	-2.46445200
C	2.22013300	-2.16232600	-0.33171800
C	2.41452700	-1.48977200	0.90180800
C	3.61973300	-1.73375700	1.59966400
C	4.58857200	-2.59894100	1.07600100
C	4.36786100	-3.23946000	-0.15506900
C	3.17068800	-3.03302200	-0.86681000
C	1.36188600	-0.61524800	1.38284200
C	-2.68697800	0.09177200	2.15149900
C	-2.97716800	-1.14975400	1.56294700
C	-4.42646300	-1.09969000	1.94773300
C	-4.10596800	0.30739100	2.60628300
H	-5.14611500	0.98143200	-0.30005200

H	-3.22999900	-1.54458000	-3.22974700
H	-2.14754600	3.12562300	0.29690300
H	-3.73300700	2.64408300	0.94713100
H	-3.65307200	3.62144700	-0.54185600
H	-5.45439200	-2.09208300	-2.50231500
H	-6.45402600	-0.75603800	-1.85434700
H	-5.58754200	-1.82980100	-0.73465400
H	-0.67845300	0.59455200	-4.11864800
H	-1.02137500	-1.14115800	-3.95258300
H	0.08359200	-0.32917700	-2.80456600
H	-0.89741900	3.85681800	-2.08031700
H	-0.25048900	2.68081700	-3.26967000
H	1.93660700	3.28458100	-2.44085400
H	1.24312700	4.06637800	-0.98722900
H	4.58105400	2.07343000	2.47926200
H	5.52294200	-0.06913600	-1.15150900
H	1.71764900	3.79293500	1.27459800
H	2.50795800	3.19244500	2.75560800
H	1.14563700	2.29450500	2.03001800
H	7.38482700	0.96824000	0.64735900
H	6.66791400	-0.50485500	1.33698800
H	6.70956800	0.99973500	2.29976800
H	2.26737900	-0.28121000	-2.39348300
H	3.97297700	-0.23455300	-2.92264600
H	2.91628600	1.18618900	-3.15397200
H	3.77901900	-1.22872800	2.55785700
H	5.51329000	-2.78599000	1.63170000
H	5.12281100	-3.91758900	-0.56626100
H	2.99776300	-3.54466800	-1.81749100
H	1.48356300	-0.20508400	2.39985500
C	0.40987600	-2.90920100	-1.76056000
H	0.94389900	-2.99158400	-2.72267000
H	0.43593500	-3.86669600	-1.21497200
H	-0.62889100	-2.59550300	-1.92483300

TS1_L1

E(BP86)= -2433.62393383 Hartree

Ru	-0.18280700	0.28216600	-0.62588400
S	-1.89162600	0.52217200	-2.08615200
S	-1.45401900	1.49894100	0.80066300
O	1.45486000	1.45875000	1.70839100
N	-0.71911100	-2.39166200	0.62889300
N	1.45489400	-2.11761600	0.41332700
C	-2.11373700	-2.05920200	0.67296000

C	-2.90201700	-2.33617500	-0.46239000
C	-4.22794400	-1.87602200	-0.47179800
C	-4.76699100	-1.15496200	0.60799300
C	-3.96617200	-0.95007500	1.74543700
C	-2.63443200	-1.38821300	1.79910900
C	-2.30595000	-3.03764500	-1.65789100
C	-6.14868100	-0.55117500	0.52116500
C	-1.76702800	-1.10444000	3.00186300
C	-0.15985900	-3.58368800	1.29740900
C	1.32311700	-3.51597900	0.88712800
C	0.24168500	-1.52310800	0.19776400
C	2.71518200	-1.63914000	-0.06663800
C	3.00435200	-1.70789100	-1.44772900
C	4.24116600	-1.20793100	-1.88841100
C	5.18150600	-0.66223800	-0.99644800
C	4.86884000	-0.63734600	0.37393100
C	3.64574900	-1.12359700	0.86095900
C	1.99240900	-2.25976500	-2.42173500
C	6.48699800	-0.08460500	-1.49241300
C	3.32375800	-1.08029800	2.33513700
C	2.51500500	1.97936100	1.03088200
C	2.50462500	1.78309300	-0.38810100
C	3.59650700	2.30701300	-1.12621000
C	4.65497700	2.98201000	-0.50973000
C	4.64535200	3.14825000	0.88460600
C	3.58048100	2.64996400	1.65419200
C	1.50066600	0.99176200	-1.05415200
H	-4.84168900	-2.04649200	-1.36445900
H	-4.37208300	-0.38479200	2.59304500
H	-1.60028800	-2.36527600	-2.17884800
H	-3.09099300	-3.32687500	-2.37608000
H	-1.74602200	-3.94542700	-1.36916500
H	-6.80828000	-1.13630100	-0.14304200
H	-6.08313800	0.47401600	0.11064000
H	-6.62682500	-0.48244800	1.51392700
H	-1.63844000	-2.00160900	3.63889800
H	-2.21468500	-0.31336100	3.62510000
H	-0.76510200	-0.76385700	2.68822800
H	-0.66778900	-4.49879100	0.95021800
H	-0.29509300	-3.50472500	2.39353400
H	2.01563900	-3.71159300	1.72223700
H	1.56604500	-4.21519100	0.06322800
H	4.47234600	-1.23838800	-2.96059700
H	5.58217200	-0.19700800	1.08078900

H	1.64473600	-3.26833000	-2.13309400
H	2.41421000	-2.32087400	-3.43861000
H	1.08989100	-1.61729500	-2.45856600
H	7.35359000	-0.53039400	-0.97092700
H	6.51838300	1.00486100	-1.30653100
H	6.61869700	-0.24962100	-2.57520100
H	2.25818700	-0.84932700	2.49356700
H	3.93193100	-0.31179600	2.84109500
H	3.53717800	-2.04797400	2.82982300
H	3.59594700	2.15625400	-2.21147000
H	5.47630200	3.38587400	-1.11099100
H	5.46460300	3.67715200	1.38395800
H	3.58525800	2.78859700	2.73867400
H	1.67983200	0.85650200	-2.14223900
C	1.27895200	1.81629800	3.07856000
H	2.06203400	1.36885600	3.72115600
H	1.27934900	2.91474000	3.20257100
H	0.29291200	1.41562000	3.35492700
C	-3.13894500	1.56682900	-1.36392200
C	-4.31587000	1.91968000	-2.05282000
C	-2.94439200	1.98694500	-0.03321400
C	-5.29721800	2.68431100	-1.40807800
H	-4.45717200	1.58452900	-3.08721500
C	-3.93499500	2.75463600	0.61294600
C	-5.10630300	3.10034000	-0.07302500
H	-6.21449000	2.95589100	-1.94226700
H	-3.78098200	3.07051700	1.65187200
H	-5.87645900	3.69418800	0.43188800

2_L1

E(BP86)= -2433.62950918 Hartree

Ru	-0.16328200	0.17088800	-0.85790800
S	-2.02030600	0.95666200	-2.03043600
S	-0.80387900	1.49391900	0.86981000
O	2.09982500	2.14400300	0.97111200
N	-1.15195600	-2.10244600	0.72914800
N	1.04792200	-2.24963800	0.54944900
C	-2.50574100	-1.74623600	0.39538700
C	-3.01660100	-2.07339700	-0.87890200
C	-4.33371200	-1.68915700	-1.17936500
C	-5.13693400	-1.00700900	-0.25071500
C	-4.60748700	-0.73738200	1.02348000
C	-3.29924800	-1.10358900	1.37289800
C	-2.15610700	-2.74578500	-1.91969300

C	-6.53973000	-0.56690600	-0.60277800
C	-2.74190000	-0.78543300	2.73692000
C	-0.85011800	-3.42792200	1.30876400
C	0.68863500	-3.41538000	1.38982400
C	-0.04239200	-1.48512900	0.22581600
C	2.40612500	-1.79458200	0.52808100
C	3.25184600	-2.23246300	-0.51200300
C	4.58960100	-1.80447800	-0.50265100
C	5.08950800	-0.96706000	0.51025600
C	4.21600000	-0.55981600	1.53583700
C	2.87108100	-0.95892100	1.56866500
C	2.70978200	-3.11261700	-1.61336800
C	6.51781600	-0.47637400	0.47798800
C	1.93766000	-0.48784300	2.65613200
C	3.07730000	2.09028000	0.03579100
C	2.83088200	1.22159200	-1.07488800
C	3.84372900	1.11845200	-2.06245500
C	5.03574900	1.84340400	-1.98655100
C	5.24410000	2.70315800	-0.89492600
C	4.27639600	2.82313400	0.11440700
C	1.63513300	0.42791400	-1.20750900
H	-4.73206800	-1.90770400	-2.17759700
H	-5.21602900	-0.19468400	1.75591900
H	-1.43613500	-2.01402000	-2.33731200
H	-2.77018700	-3.13121000	-2.75048000
H	-1.56528600	-3.58313400	-1.50750600
H	-7.29750700	-1.10681700	-0.00399600
H	-6.76228800	-0.74408100	-1.66866400
H	-6.66443800	0.51148300	-0.40124400
H	-2.38398400	-1.69091500	3.26218200
H	-3.50808000	-0.30652200	3.36810700
H	-1.88137400	-0.09676000	2.64108600
H	-1.23048200	-4.22483400	0.64105600
H	-1.33651800	-3.54241600	2.29204500
H	1.05525600	-3.26427500	2.42228900
H	1.15089900	-4.33586000	0.99404700
H	5.25727100	-2.12620500	-1.31130100
H	4.59108400	0.09907300	2.32898000
H	2.38561500	-4.09873600	-1.23123800
H	3.47225500	-3.28811900	-2.39051700
H	1.82528400	-2.65286000	-2.09047100
H	6.93602100	-0.37726300	1.49507300
H	6.56611600	0.51941700	-0.00014900
H	7.16823100	-1.15625400	-0.09878100

H	1.05321300	0.01356400	2.22662800
H	2.44797800	0.22698200	3.32217000
H	1.57283600	-1.32284200	3.28397500
H	3.66374800	0.44394500	-2.90743400
H	5.79355200	1.74564500	-2.77031900
H	6.16810400	3.28752100	-0.82077700
H	4.46024200	3.48786900	0.96198700
H	1.67291300	-0.23467000	-2.13183100
C	2.24556300	3.04859700	2.06325500
H	3.10915400	2.77484000	2.70074200
H	2.36334800	4.08968700	1.70888800
H	1.31095600	2.95769400	2.63464300
C	-2.97091400	1.83616300	-0.82049100
C	-4.26960800	2.29749500	-1.11945700
C	-2.46009300	2.00513300	0.48906500
C	-5.06465800	2.87601500	-0.12193300
C	-3.26550800	2.58773500	1.48988000
C	-4.56455900	3.01370700	1.18850800
H	-6.07753200	3.21825200	-0.36329000
H	-5.18895900	3.45506800	1.97349900
H	-4.65581200	2.17095300	-2.13708600
H	-2.86599100	2.69058000	2.50597300

3_L1

E(BP86)= -2433.61463231 Hartree

Ru	-0.67245200	0.00592500	0.43639900
O	1.41662100	2.89605600	2.26752600
N	-2.01832400	-2.44762100	-0.20444900
N	0.10990300	-2.99319800	-0.20735000
C	-3.13288900	-1.54731100	-0.07909500
C	-3.65327000	-0.90624500	-1.22523800
C	-4.66240400	0.05410100	-1.03528900
C	-5.13598800	0.39450100	0.24161500
C	-4.61189200	-0.28408000	1.35883500
C	-3.61032100	-1.25525100	1.22282300
C	-3.07161300	-1.14846500	-2.59465300
C	-6.14942100	1.50145900	0.42027700
C	-3.01401800	-1.93888200	2.43348700
C	-2.05900900	-3.86415300	-0.61455500
C	-0.58258900	-4.28946800	-0.41690600
C	-0.75831700	-1.96970100	-0.01810800
C	1.53466000	-2.90589200	-0.10356800
C	2.29586600	-2.82675200	-1.29028500
C	3.69425600	-2.73919000	-1.17291700

C	4.33019300	-2.69669800	0.08074000
C	3.53730200	-2.79141400	1.23894800
C	2.13940900	-2.90670300	1.17188700
C	1.62026800	-2.75303600	-2.63866600
C	5.82216100	-2.47884600	0.18528400
C	1.29983400	-2.98762500	2.42399000
C	2.30988000	2.38933700	1.36158500
C	2.06163500	1.04932100	0.94254000
C	2.92233800	0.47794700	-0.01383000
C	4.01105800	1.18754400	-0.53125800
C	4.23259400	2.51174500	-0.11905400
C	3.38276100	3.11879900	0.81779300
C	0.84008800	0.39494800	1.41150100
H	-5.05879100	0.57931400	-1.91258800
H	-4.97513700	-0.03163700	2.36249800
H	-2.09078100	-0.63527100	-2.67301700
H	-3.73140000	-0.73916000	-3.37750100
H	-2.90861100	-2.21886500	-2.81007000
H	-6.79471900	1.32609900	1.29864100
H	-6.79429600	1.61008500	-0.46861600
H	-5.63335300	2.46761700	0.57517900
H	-3.00055900	-3.03831900	2.32268700
H	-3.58269500	-1.68865000	3.34403000
H	-1.96385600	-1.62727500	2.59521000
H	-2.38834800	-3.96203400	-1.66638500
H	-2.75853000	-4.43484900	0.01995200
H	-0.44410300	-4.93660300	0.47018000
H	-0.16483800	-4.81437600	-1.29195100
H	4.29754300	-2.66084700	-2.08571200
H	4.01884200	-2.76065500	2.22400200
H	0.93158300	-3.59924400	-2.81588800
H	2.36621000	-2.74993000	-3.45051500
H	1.02670000	-1.82356900	-2.71532600
H	6.25247500	-3.00422000	1.05560300
H	6.03990900	-1.40091300	0.31080800
H	6.34912800	-2.82119700	-0.72183900
H	0.70585500	-2.06376300	2.54335400
H	1.93408000	-3.11100600	3.31725900
H	0.58591300	-3.83057700	2.38948100
H	2.69803500	-0.52952100	-0.36037900
H	4.66429100	0.71787400	-1.27447000
H	5.06463800	3.08950100	-0.53727100
H	3.55063700	4.15829900	1.11014100
H	0.63434100	0.48545900	2.50495200

C	1.42296300	4.30914000	2.47039600
H	2.35012200	4.64810200	2.97425400
H	1.30202700	4.83833800	1.50711100
H	0.55872800	4.51775100	3.11805700
C	-0.64131000	3.00083400	-0.61922000
C	-0.55968500	4.40657800	-0.54770100
C	0.35547000	5.10951800	-1.34507100
C	1.20206900	4.41275000	-2.22810900
C	1.11830000	3.01827800	-2.32316400
C	0.18903200	2.30728700	-1.53842100
H	-1.21034500	4.93978200	0.15529400
H	0.41936900	6.20088700	-1.26598200
H	1.93796500	4.95613200	-2.83111100
H	1.78767800	2.46081700	-2.98775100
S	0.07619100	0.53785500	-1.66597500
S	-1.72858300	2.08819200	0.45528500

TS2_L1

E(BP86)= -2433.59916463 Haetree

Ru	0.92862000	-0.21294400	0.43704600
O	-3.14630200	-0.44786200	2.64605000
N	2.61118900	2.01556100	-0.26983100
N	0.52713600	2.71344500	-0.45681400
C	3.57402500	1.05109100	0.16333400
C	4.61906900	0.65861100	-0.69773400
C	5.40363700	-0.45028700	-0.33766100
C	5.14288800	-1.20053300	0.82680300
C	4.10514500	-0.78681100	1.67372500
C	3.29843600	0.33532900	1.37292100
C	4.83095600	1.36840100	-2.01388200
C	5.94224500	-2.44646100	1.13659100
C	2.31114700	0.84940700	2.40208300
C	2.76592200	3.47735900	-0.39123900
C	1.33345500	3.90464100	-0.80499200
C	1.29505600	1.62132800	-0.20500400
C	-0.90389400	2.68541800	-0.51542500
C	-1.54364700	2.39212800	-1.73752800
C	-2.94767900	2.37342000	-1.75692200
C	-3.71122600	2.61087200	-0.59957300
C	-3.03650500	2.88677000	0.60176700
C	-1.63421000	2.93241500	0.66611700
C	-0.73966200	2.02646600	-2.96077900
C	-5.21873000	2.52160800	-0.64430300
C	-0.91870200	3.21601900	1.96524500

C	-3.36789100	-0.62779800	1.30550000
C	-2.21376100	-0.52322100	0.45793900
C	-2.41329400	-0.67927000	-0.93101100
C	-3.67133300	-0.96899700	-1.47193700
C	-4.77453700	-1.10120100	-0.62009600
C	-4.63147300	-0.91818900	0.76783300
C	-0.90911800	-0.29185100	1.06279600
H	6.21109600	-0.76515900	-1.01001300
H	3.90107500	-1.34721100	2.59377200
H	3.86815100	1.49654200	-2.54127600
H	5.50888400	0.79365700	-2.66592400
H	5.27245500	2.37531400	-1.88211800
H	5.93703700	-2.67264100	2.21676800
H	6.99228800	-2.34856800	0.80952200
H	5.51526600	-3.32424700	0.61533400
H	2.31034600	1.95201300	2.45889400
H	2.54321600	0.43311300	3.39671600
H	1.21167800	0.58331600	2.25515200
H	3.52190300	3.74890700	-1.14631400
H	3.06944400	3.91656000	0.57961000
H	0.97473500	4.79304400	-0.25855000
H	1.26243500	4.11431900	-1.88983500
H	-3.45901900	2.13616100	-2.69767100
H	-3.61597100	3.06390300	1.51619500
H	0.03821000	2.77542900	-3.19530300
H	-1.39162000	1.92613400	-3.84451200
H	-0.22384800	1.05873300	-2.80133600
H	-5.68128500	3.02159200	0.22407300
H	-5.53572300	1.46253600	-0.63157900
H	-5.62600000	2.97897600	-1.56346300
H	-0.24158000	2.38452100	2.22646400
H	-1.63803700	3.34857800	2.79006900
H	-0.29778000	4.12967200	1.90480800
H	-1.54217700	-0.55032900	-1.57566300
H	-3.78355700	-1.09763900	-2.55296000
H	-5.76318500	-1.34575200	-1.02573700
H	-5.50621500	-1.01634000	1.41537700
H	-1.02946800	0.00506700	2.12174400
C	-4.26691900	-0.54166900	3.52156900
H	-5.03712200	0.21638100	3.27812100
H	-4.72432600	-1.54920700	3.48763100
H	-3.87203100	-0.35364200	4.53104600
C	-0.43277500	-3.18103500	-0.09741600
C	-0.11051500	-2.68396300	-1.39027600

S	0.78100900	-1.15794300	-1.63818000
S	0.10898700	-2.38667800	1.39153100
C	-1.21759900	-4.35086100	0.01600600
C	-0.55906500	-3.39113000	-2.52825500
C	-1.64908200	-5.04358600	-1.11981000
H	-2.25518500	-5.94949200	-1.00954300
C	-1.31117800	-4.56316900	-2.39891700
H	-1.65008900	-5.09352400	-3.29604600
H	-1.47848500	-4.71067400	1.01753100
H	-0.31772800	-2.99420000	-3.52130900

4_L1

E(BP86)= -2433.60477698 Hartree

Ru	-1.00762300	0.16424100	0.46210900
O	3.22433800	0.22201400	2.48103600
N	-2.38494400	-2.15077100	-0.48823400
N	-0.23159300	-2.60323600	-0.64600700
C	-3.44552900	-1.35045200	0.04138100
C	-4.53902200	-0.99593300	-0.77623600
C	-5.45717300	-0.04841500	-0.29479700
C	-5.28805400	0.58534300	0.95403100
C	-4.19802700	0.21540400	1.75295200
C	-3.25530700	-0.75385500	1.33181700
C	-4.66291300	-1.56844400	-2.16817900
C	-6.24631600	1.66570800	1.40399600
C	-2.21133200	-1.26222800	2.30675000
C	-2.37302500	-3.60530500	-0.72941300
C	-0.89573100	-3.82944400	-1.14205200
C	-1.11987000	-1.62312800	-0.33525200
C	1.19248400	-2.45293100	-0.62629500
C	1.86140900	-2.00906400	-1.78506400
C	3.26294000	-1.92809400	-1.74669600
C	3.99519300	-2.26218900	-0.59452000
C	3.29015400	-2.66802800	0.55189700
C	1.89015300	-2.76852900	0.55875900
C	1.08258900	-1.56294900	-2.99790500
C	5.50575700	-2.20734300	-0.60125700
C	1.14658700	-3.16670900	1.81095200
C	3.38528700	0.61522500	1.17044000
C	2.18477600	0.76220000	0.41153400
C	2.31977900	1.11844300	-0.94241900
C	3.57008200	1.38087800	-1.52145400
C	4.72953700	1.27186800	-0.74591700
C	4.64191800	0.87269400	0.59850900

C	0.88288500	0.58099300	1.10251300
H	-6.30397400	0.23644500	-0.93130800
H	-4.06348800	0.68257500	2.73596300
H	-3.69587700	-1.49669700	-2.69841500
H	-5.42128000	-1.02230000	-2.75277200
H	-4.95609200	-2.63618800	-2.15965300
H	-6.21119700	1.80768000	2.49782600
H	-7.28750900	1.42955000	1.12113800
H	-5.99211900	2.63641100	0.93727700
H	-2.09922200	-2.35977800	2.25766900
H	-2.47264700	-0.96882600	3.33705900
H	-1.13692300	-0.88639400	2.18330000
H	-3.08132700	-3.89770300	-1.52214100
H	-2.63792000	-4.15598800	0.19538700
H	-0.44965400	-4.72805200	-0.68399200
H	-0.78356200	-3.90857100	-2.24093100
H	3.79592900	-1.56853200	-2.63453500
H	3.84336100	-2.90655600	1.46892600
H	0.42315100	-2.35873100	-3.39175400
H	1.76327400	-1.25654600	-3.80942300
H	0.43731000	-0.70002400	-2.74363300
H	5.90875100	-2.07832600	0.41796800
H	5.86865300	-1.36690700	-1.21631900
H	5.93875300	-3.13858000	-1.01526900
H	0.54309100	-2.32102100	2.18573800
H	1.84821300	-3.46567300	2.60728900
H	0.44830000	-4.00561200	1.63549700
H	1.41469500	1.15993700	-1.55097100
H	3.62926100	1.66705200	-2.57670700
H	5.71404800	1.48365300	-1.17880000
H	5.55535100	0.76936700	1.18977200
H	1.06805300	0.09899600	2.07878500
C	4.40167300	-0.03696000	3.23666900
H	5.02194900	-0.82361200	2.76253800
H	5.01507600	0.87618000	3.36690800
H	4.05535700	-0.38548400	4.22146800
C	0.17758300	3.24792800	0.13766900
C	-0.30999600	2.89658300	-1.14897000
S	-1.02446300	1.31246300	-1.51702300
S	-0.04505000	2.18708200	1.56206400
C	0.81609200	4.48532400	0.34749700
C	-0.15421500	3.83446100	-2.19711500
C	0.95616300	5.40262900	-0.70092800
H	1.45237000	6.36321100	-0.52815400

C	0.45956800	5.07092100	-1.97512700
H	0.56103500	5.77892200	-2.80563400
H	1.19911400	4.71932300	1.34687100
H	-0.52021500	3.56980100	-3.19566500

Cat._L2

E(BP86)= -3352.98991131 Hartree

Ru	-0.12432600	-0.24353000	-0.27331600
S	1.02341500	1.60586800	-1.00948500
S	1.67430200	-1.55634400	-0.90071600
O	-1.38049800	-2.13698300	0.10852800
N	0.08673300	0.99689500	2.36816300
N	-1.98361300	1.29258000	1.67282400
C	1.34379000	0.29856700	2.41782800
C	2.52641400	0.96263500	2.02544500
C	3.69407100	0.19267100	1.88764900
C	3.71954200	-1.18066100	2.17920600
C	2.54668300	-1.78312200	2.67332000
C	1.34859800	-1.06678600	2.79609500
C	2.56648200	2.45401900	1.80521800
C	4.96751900	-1.99737900	1.94438000
C	0.09870000	-1.73101100	3.32890300
C	-0.56662700	1.62504700	3.53315400
C	-1.93201400	2.04893200	2.94628300
C	-0.78121500	0.75145500	1.34360800
C	-3.15637000	1.28108900	0.85414400
C	-3.32478200	2.26634300	-0.14029000
C	-4.48471300	2.20463400	-0.93398900
C	-5.45665100	1.20610600	-0.75225300
C	-5.25538000	0.24625300	0.25709000
C	-4.11093100	0.26162900	1.06647100
C	-2.27259500	3.32364300	-0.36796500
C	-6.67898400	1.13455400	-1.63837500
C	-3.87631200	-0.80380800	2.11125000
C	-2.48266800	-2.14513800	-0.74082700
C	-2.56235900	-1.00394300	-1.57945400
C	-3.65571500	-0.92541400	-2.47241100
C	-4.62974000	-1.93168800	-2.50615300
C	-4.52436100	-3.04280000	-1.65233400
C	-3.43883300	-3.16160000	-0.76328200
C	-1.52913500	0.00991900	-1.47047300
H	4.60358000	0.68191500	1.51937000
H	2.56141100	-2.84635300	2.94417600
H	1.57299900	2.85464100	1.55820100

H	3.24496800	2.71391900	0.97747500
H	2.93848300	2.96159000	2.71748700
H	5.87696300	-1.37623300	2.01234000
H	4.94660500	-2.44157800	0.93204000
H	5.05564300	-2.82508900	2.67004400
H	-0.17563200	-1.34171200	4.32803100
H	0.24844100	-2.81839800	3.43444800
H	-0.76834800	-1.56412500	2.66666400
H	0.02854600	2.47847800	3.89824100
H	-0.67302900	0.89433500	4.35794600
H	-2.78531700	1.78059400	3.59145700
H	-1.98072900	3.13499900	2.74059500
H	-4.62590400	2.95538600	-1.72136300
H	-5.99190400	-0.55430400	0.39470000
H	-2.07061400	3.91029800	0.54695400
H	-2.58524900	4.02746900	-1.15675600
H	-1.31281500	2.87050600	-0.67446800
H	-7.61262300	1.19874000	-1.04988400
H	-6.70582700	0.17369500	-2.18500200
H	-6.68949300	1.94964200	-2.38138400
H	-2.92507000	-1.33108900	1.92354800
H	-4.69050100	-1.54661700	2.09977100
H	-3.81557700	-0.38012100	3.13137100
H	-3.72741200	-0.05424700	-3.13182500
H	-5.46651600	-1.86037000	-3.20904200
H	-5.28126300	-3.83363000	-1.68017600
H	-3.35202800	-4.03257200	-0.10772200
H	-1.55738600	0.82317300	-2.21541800
C	-0.82608400	-3.41393700	0.49703300
H	-1.46900900	-3.89400200	1.25524300
H	-0.72134500	-4.05927000	-0.39056900
H	0.16228100	-3.18838000	0.91844900
C	2.62882100	0.99756500	-1.43116300
C	3.67283200	1.88721900	-1.77584000
C	2.91320700	-0.39858500	-1.40936000
C	4.96086400	1.44299000	-2.09018400
C	4.21041200	-0.82918600	-1.76115300
C	5.23454600	0.06735100	-2.08522900
H	5.74012800	2.16709800	-2.34260400
H	6.23079700	-0.30675300	-2.33472400
Cl	3.36027200	3.62651000	-1.80739600
Cl	4.58559100	-2.55677900	-1.79152600

TS1_L2

E(BP86)= -3352.95960662 Hartree

Ru	0.13992800	-0.00214500	0.58110700
S	-1.61844900	0.17043200	1.98311400
S	-1.17728600	-1.34030200	-0.66852700
O	1.69324000	-1.75520400	-1.39513500
N	-0.09189500	2.45822300	-1.10597600
N	2.03824600	2.06060500	-0.71546200
C	-1.50511600	2.21950400	-1.18687900
C	-2.32916400	2.73547500	-0.16509200
C	-3.68767600	2.38428400	-0.17493300
C	-4.22586700	1.54223800	-1.16455700
C	-3.38092700	1.08340000	-2.19012700
C	-2.01461500	1.40426100	-2.21908000
C	-1.74670000	3.58706300	0.93686100
C	-5.66488500	1.08890100	-1.08948100
C	-1.10651000	0.84841900	-3.28951300
C	0.59545400	3.49040500	-1.90858900
C	2.05111900	3.36656800	-1.41667600
C	0.77240300	1.60303500	-0.48957400
C	3.23518800	1.53870000	-0.12983000
C	3.52030200	1.81030200	1.22597000
C	4.69622300	1.26901100	1.77279900
C	5.57909400	0.48769600	1.00636000
C	5.26798600	0.25339800	-0.34481900
C	4.10530500	0.77226400	-0.93443000
C	2.56173200	2.61655400	2.06825500
C	6.83092000	-0.10203300	1.61457200
C	3.77103000	0.49585200	-2.38004300
C	2.69544000	-2.21256800	-0.59605600
C	2.67514700	-1.74342600	0.75714100
C	3.70315600	-2.20123000	1.62085400
C	4.71197700	-3.06445000	1.18206800
C	4.71483300	-3.49634900	-0.15411800
C	3.71146700	-3.07350700	-1.04213500
C	1.72963600	-0.76183200	1.22658500
H	-4.33319900	2.74337000	0.63537300
H	-3.78330900	0.41269800	-2.95860000
H	-1.00988400	3.00986900	1.52372400
H	-2.53630200	3.92590300	1.62707000
H	-1.22871900	4.47993000	0.53947600
H	-6.31052400	1.85820100	-0.63124700
H	-5.74136900	0.17740900	-0.46821300
H	-6.06707000	0.84429400	-2.08768500

H	-0.86720700	1.60541300	-4.06179000
H	-1.58289500	-0.00706900	-3.79517100
H	-0.15578100	0.49798400	-2.85157100
H	0.15576600	4.48416100	-1.72175900
H	0.49566400	3.26190900	-2.98714000
H	2.78883900	3.36103000	-2.23574700
H	2.32811700	4.16932700	-0.70621900
H	4.92383900	1.45649700	2.82960200
H	5.92987000	-0.37958800	-0.94740700
H	2.35077900	3.60670600	1.62436400
H	2.96400400	2.77599300	3.08227600
H	1.58593000	2.09991800	2.15998400
H	7.74276700	0.35883800	1.19060700
H	6.88661200	-1.18658600	1.41307700
H	6.85774200	0.04516900	2.70752300
H	2.69860000	0.26663900	-2.48994900
H	4.35611900	-0.35979400	-2.75628900
H	3.99776400	1.36382800	-3.02927900
H	3.69480400	-1.84494900	2.65682200
H	5.48515700	-3.40630800	1.87777500
H	5.49535700	-4.17581900	-0.51371300
H	3.72418800	-3.42021700	-2.07880900
H	1.87989100	-0.45825700	2.28395000
C	1.51244200	-2.35614400	-2.67868200
H	2.33666100	-2.09349000	-3.36971300
H	1.43383300	-3.45477000	-2.59026800
H	0.56228700	-1.95041900	-3.05483700
C	-2.94218000	-0.84905300	1.37414300
C	-4.18877100	-0.96177200	2.01888600
C	-2.74214300	-1.51271400	0.14285100
C	-5.23094700	-1.71794400	1.47000300
C	-3.80291300	-2.25696900	-0.41064800
C	-5.03582200	-2.37123600	0.23882900
H	-6.18929700	-1.78767500	1.99169500
H	-5.84094600	-2.95529300	-0.21534900
Cl	-3.58016200	-3.04150100	-1.97773200
Cl	-4.45767300	-0.11140000	3.54073300

2_L2

E(BP86)= -3352.96375089 Hartree

Ru	-0.21132100	-0.26965000	0.91760000
S	1.74916500	-0.51758500	2.12195600
S	0.75401400	1.52264500	-0.06944400
O	-1.87882300	2.12311100	-0.85590100

N	0.37642100	-1.70796000	-1.59810600
N	-1.80776900	-1.64778200	-1.29736500
C	1.79316500	-1.56640000	-1.41082400
C	2.44913300	-2.46277800	-0.53601500
C	3.83011100	-2.31089800	-0.34781900
C	4.56481900	-1.31628000	-1.01987300
C	3.88587700	-0.47198600	-1.91291100
C	2.50113300	-0.58164700	-2.13166000
C	1.67572000	-3.53495900	0.19174000
C	6.05381000	-1.18183600	-0.79656600
C	1.80579100	0.33105300	-3.11288000
C	-0.15720600	-2.36451000	-2.80933700
C	-1.64582700	-2.54370200	-2.46279100
C	-0.60548800	-1.25905900	-0.76061700
C	-3.08665500	-1.51195100	-0.67721200
C	-3.38294500	-2.26328800	0.48368000
C	-4.63793300	-2.08105000	1.08801800
C	-5.59480000	-1.19706100	0.55713600
C	-5.28134300	-0.50098800	-0.62355200
C	-4.03823100	-0.64354900	-1.25785500
C	-2.36122700	-3.20149800	1.07902400
C	-6.91806600	-0.96804800	1.25007500
C	-3.71260200	0.13816300	-2.50732200
C	-2.92748500	2.24112200	-0.00224600
C	-2.94321500	1.33492100	1.10745100
C	-4.04564400	1.41149500	1.99742700
C	-5.08524400	2.32864500	1.82058500
C	-5.04635100	3.20106200	0.72042300
C	-3.97630100	3.16024800	-0.18728200
C	-1.95800000	0.29542300	1.29220200
H	4.34357900	-2.97410400	0.35828600
H	4.44030200	0.31712000	-2.43417900
H	1.00942100	-3.08146400	0.94849800
H	2.35860200	-4.22613500	0.71240100
H	1.04118400	-4.12359700	-0.49665400
H	6.61427900	-1.96328000	-1.34539100
H	6.30411900	-1.28618700	0.27352700
H	6.42028500	-0.19988200	-1.13840200
H	1.78124000	-0.11312800	-4.12797800
H	2.33142100	1.29685500	-3.18297400
H	0.77137500	0.53968300	-2.79561800
H	0.36584900	-3.31857600	-2.98883300
H	-0.00483100	-1.71270800	-3.69020100
H	-2.31971700	-2.24316100	-3.28189200

H	-1.89359600	-3.58457500	-2.17549000
H	-4.87215700	-2.64069800	2.00213800
H	-6.00975500	0.20429200	-1.04140500
H	-1.94016200	-3.88976600	0.32470800
H	-2.80137800	-3.80304600	1.89121200
H	-1.49542900	-2.64807400	1.49969900
H	-7.76990500	-1.12633300	0.56403300
H	-6.98391200	0.07357400	1.61595000
H	-7.04636000	-1.64129900	2.11438600
H	-2.64598700	0.41254600	-2.52312900
H	-4.31376600	1.06190600	-2.55080400
H	-3.93320200	-0.44301000	-3.42390100
H	-4.06557600	0.71155900	2.84034800
H	-5.91456500	2.37037000	2.53410900
H	-5.85280900	3.92570500	0.56246400
H	-3.96506800	3.84536700	-1.03890800
H	-2.26985800	-0.41332300	2.10636700
C	-1.69838900	3.11974500	-1.86383300
H	-2.48589300	3.05439300	-2.63928100
H	-1.69095900	4.13295400	-1.42258100
H	-0.71380900	2.90511900	-2.30347700
C	2.90669700	0.61266500	1.41227300
C	4.27631400	0.61041400	1.75085400
C	2.45298800	1.51882600	0.41767700
C	5.18977800	1.47846300	1.14467400
C	3.38603500	2.39488300	-0.17710400
C	4.73822300	2.38496200	0.17099200
H	6.24596400	1.44153900	1.42345600
H	5.43404100	3.07318400	-0.31658200
Cl	2.84429500	3.53055900	-1.42237600
Cl	4.88420400	-0.54517500	2.93577700

3_L2

E(BP86)= -3352.95044468 Hartree

Ru	0.43918500	-0.70592800	-0.52929100
O	0.40623200	2.75852200	-2.55828900
N	0.16965100	-3.44510500	0.28611500
N	-1.90252900	-2.71824500	0.17335400
C	1.59942100	-3.28922400	0.23023800
C	2.32798500	-2.97883300	1.40113800
C	3.69604900	-2.68845600	1.26310400
C	4.33441300	-2.67711000	0.01195400
C	3.58476600	-3.01957400	-1.12834000
C	2.21770700	-3.32347000	-1.04488800

C	1.64768300	-2.85791200	2.74169400
C	5.77740400	-2.24728000	-0.11496800
C	1.41443200	-3.63313800	-2.28941300
C	-0.59960200	-4.57935600	0.83519000
C	-2.04726500	-4.16340300	0.48221500
C	-0.60827800	-2.36829600	-0.01397500
C	-3.02997700	-1.86312400	-0.04345100
C	-3.66740800	-1.28947400	1.07852700
C	-4.76734400	-0.44398500	0.85082300
C	-5.20938000	-0.13782900	-0.44848200
C	-4.55490600	-0.73894500	-1.53892300
C	-3.47022800	-1.61310100	-1.36116300
C	-3.12854000	-1.50095200	2.47314100
C	-6.31330000	0.87004800	-0.67130600
C	-2.77151500	-2.24106500	-2.54336400
C	-0.65176300	2.89369000	-1.70089000
C	-1.21312100	1.67164300	-1.22326800
C	-2.27358900	1.73908500	-0.29920600
C	-2.78822500	2.96535100	0.13195000
C	-2.21529000	4.15835900	-0.33637500
C	-1.14723100	4.12947800	-1.24600300
C	-0.55440200	0.42119300	-1.59482900
H	4.26712000	-2.41688400	2.15890300
H	4.06934800	-3.01889600	-2.11213100
H	0.90363000	-2.03856500	2.71514100
H	2.38112500	-2.61273600	3.52702600
H	1.12996800	-3.78629300	3.04451900
H	6.27199500	-2.72664600	-0.97748000
H	6.35563500	-2.48518800	0.79437100
H	5.83223600	-1.15280300	-0.26613900
H	0.78585600	-4.53214300	-2.16061900
H	2.07969900	-3.78995600	-3.15419100
H	0.72522000	-2.80396200	-2.54292800
H	-0.44747900	-4.66563900	1.92756100
H	-0.29529000	-5.52769200	0.36242400
H	-2.43394700	-4.69844300	-0.40661900
H	-2.75545300	-4.31537700	1.31265300
H	-5.26218000	0.02199800	1.71168500
H	-4.89064900	-0.51277600	-2.55832300
H	-2.96078100	-2.56696000	2.70919600
H	-3.82060100	-1.09039000	3.22665500
H	-2.15831000	-0.98197400	2.58400700
H	-6.89469900	0.64594200	-1.58241900
H	-5.88301100	1.88231100	-0.79524300

H	-7.00963600	0.90842500	0.18404600
H	-1.74974100	-1.83402200	-2.64599600
H	-3.32027400	-2.03842300	-3.47777500
H	-2.67547900	-3.33658800	-2.43296500
H	-2.66750200	0.80345400	0.09344900
H	-3.60454800	2.98756300	0.86066300
H	-2.58809900	5.12588600	0.01780600
H	-0.69653100	5.06571600	-1.58415600
H	-0.27925000	0.32345000	-2.67228000
C	1.15068800	3.93548800	-2.87391300
H	0.55399800	4.64420100	-3.48187000
H	1.50060400	4.43589200	-1.95275700
H	2.01982200	3.58917700	-3.45037300
C	1.97604000	1.88145600	0.45581200
C	2.64235300	3.12116600	0.35689200
C	2.22339400	4.25179200	1.07049100
C	1.12956700	4.15059900	1.94283700
C	0.47984000	2.92080500	2.08683800
C	0.87533400	1.78040100	1.35673900
H	2.74842300	5.20232000	0.94247700
H	0.78011900	5.02082200	2.50463900
S	0.00406100	0.24508500	1.50474000
S	2.44825900	0.47639700	-0.52121900
Cl	-0.87193200	2.80586500	3.21305600
Cl	4.04330900	3.27951300	-0.70725900

TS2_L2
E(BP86)= -3352.93216678 Hartree

Ru	-1.05806300	-0.21631500	-0.57304500
O	2.99912200	-0.08335900	-2.76983300
N	-3.33079200	1.44691000	-0.01096100
N	-1.56655500	2.75762600	0.14811600
C	-3.94409500	0.19176600	-0.31218000
C	-4.79123300	-0.43125700	0.62806800
C	-5.18596200	-1.75941400	0.39482500
C	-4.72208700	-2.49257200	-0.71599800
C	-3.88676500	-1.85147100	-1.64164200
C	-3.47882100	-0.50797900	-1.47200300
C	-5.19479100	0.28723000	1.89394100
C	-5.08619800	-3.95078700	-0.88365000
C	-2.71628900	0.19676800	-2.57704200
C	-3.93558400	2.78901800	0.06423400
C	-2.70576400	3.65896400	0.43676600
C	-1.95869600	1.47491200	-0.06063400

C	-0.19657100	3.17213800	0.20715800
C	0.46574400	3.21290500	1.45166500
C	1.81686300	3.59927900	1.46465200
C	2.51587100	3.90219900	0.28327200
C	1.81990000	3.85327200	-0.93684200
C	0.46370100	3.49578000	-0.99769500
C	-0.21685200	2.74384500	2.71381400
C	3.99813400	4.19003700	0.31739700
C	-0.26378700	3.41846200	-2.31866800
C	3.22585300	0.16136300	-1.44350900
C	2.05620700	0.31630000	-0.62967700
C	2.24622300	0.54296400	0.74875700
C	3.52184800	0.60996900	1.32027500
C	4.64963600	0.43969900	0.50708100
C	4.50853000	0.22064600	-0.87480100
C	0.74136400	0.13807000	-1.24185800
H	-5.83550200	-2.25187100	1.12873400
H	-3.52946800	-2.40017900	-2.52101300
H	-4.31827400	0.77292000	2.36007300
H	-5.62582900	-0.41723200	2.62384100
H	-5.95077700	1.07460100	1.70803300
H	-5.03951400	-4.26139300	-1.94161400
H	-6.10187900	-4.16203300	-0.50590400
H	-4.38459500	-4.59542400	-0.32091200
H	-3.08429100	1.22527500	-2.73847500
H	-2.79100500	-0.37192200	-3.51857500
H	-1.59297700	0.34076600	-2.43372700
H	-4.73215500	2.83851400	0.82441100
H	-4.36972600	3.07367200	-0.91424800
H	-2.63425000	4.58087000	-0.16425200
H	-2.71008700	3.94390600	1.50609300
H	2.35082200	3.61565300	2.42263100
H	2.35126300	4.08168300	-1.86902000
H	-1.19739900	3.22629300	2.87612200
H	0.41022800	2.94662000	3.59773400
H	-0.39359400	1.65076000	2.66590700
H	4.31271400	4.81799700	-0.53409200
H	4.56300000	3.23992700	0.26174200
H	4.29492600	4.69729100	1.25191500
H	-0.54407200	2.37421100	-2.54447400
H	0.37061200	3.78995900	-3.14026600
H	-1.19910600	4.00773500	-2.31266300
H	1.35285000	0.66157400	1.36150700
H	3.62796400	0.77618700	2.39662600

H	5.65541800	0.46715900	0.94196600
H	5.39896000	0.07813000	-1.49189400
H	0.78952200	0.34747300	-2.32712500
C	4.11335000	-0.48041900	-3.56839900
H	4.86133500	0.33135900	-3.66150000
H	4.59405400	-1.38351300	-3.14837600
H	3.69907500	-0.71016300	-4.56110400
C	1.24772100	-2.45853400	0.16101300
C	0.80143300	-1.95707400	1.42384500
S	-0.59062500	-0.86029900	1.56393300
S	0.37187400	-2.10519200	-1.33620600
C	2.46161100	-3.18111900	0.11257300
C	1.56469400	-2.27449500	2.57218800
C	3.20327800	-3.47455900	1.26217200
H	4.13737800	-4.03587200	1.18099900
C	2.74180400	-3.02512000	2.50586600
H	3.30637500	-3.23284800	3.41887200
Cl	1.06891700	-1.65557300	4.14790100
Cl	3.10870900	-3.73042500	-1.43488900

4_L2

E(BP86)= -3352.93571774 Hartree

Ru	-1.10147200	-0.25221200	-0.55816100
O	3.03907500	-0.19622700	-2.83825700
N	-3.24201500	1.58272700	-0.06188200
N	-1.39152800	2.75348300	0.16940500
C	-3.95427900	0.38217200	-0.36622500
C	-4.88810000	-0.14509700	0.55107400
C	-5.42158100	-1.42143800	0.30443600
C	-5.01201700	-2.20145600	-0.79618500
C	-4.08048300	-1.65948100	-1.69274300
C	-3.53343100	-0.36770800	-1.51102900
C	-5.24438200	0.61323100	1.80802300
C	-5.54103700	-3.60621200	-0.98318200
C	-2.67702900	0.25062600	-2.59663000
C	-3.74798900	2.96517300	-0.00324600
C	-2.46985500	3.74104200	0.40670900
C	-1.86798700	1.50332200	-0.06677100
C	-0.00589800	3.10190600	0.27188500
C	0.59909200	3.17581400	1.54371900
C	1.94507100	3.57524000	1.60964000
C	2.69579900	3.85299900	0.45449400
C	2.06428400	3.74159600	-0.79645400
C	0.71432400	3.37627700	-0.91046900

C	-0.14329600	2.73941200	2.78407800
C	4.16402800	4.19577600	0.54563000
C	0.04716700	3.25747100	-2.25935800
C	3.26671400	0.10511200	-1.51695700
C	2.10228100	0.19377200	-0.69762300
C	2.28114100	0.47637000	0.66481300
C	3.55601800	0.64802700	1.22239100
C	4.68713600	0.54498800	0.40482000
C	4.54805000	0.28498800	-0.97046900
C	0.78429100	-0.12634300	-1.30596900
H	-6.14237800	-1.83745600	1.01896000
H	-3.76192300	-2.24472800	-2.56356200
H	-4.33468900	1.01946700	2.28633700
H	-5.74898100	-0.04586100	2.53334700
H	-5.92348100	1.46521800	1.60951400
H	-5.42879100	-3.94551800	-2.02719000
H	-6.60900800	-3.67754000	-0.71104200
H	-4.99175100	-4.32242600	-0.34291700
H	-3.01654100	1.27183600	-2.85066800
H	-2.68734500	-0.37481100	-3.50316800
H	-1.56650500	0.42495000	-2.37328400
H	-4.56115800	3.07451600	0.73282100
H	-4.13203600	3.28060300	-0.99328800
H	-2.30377200	4.64680300	-0.20035800
H	-2.49086600	4.04017400	1.47188700
H	2.43121400	3.63141400	2.59145900
H	2.63990700	3.93924500	-1.70913500
H	-1.11200100	3.25609000	2.90955800
H	0.45875800	2.92751100	3.68846900
H	-0.35647700	1.65355400	2.73503100
H	4.45907200	4.93457300	-0.22030000
H	4.77242100	3.28598800	0.38403600
H	4.42660000	4.60162400	1.53776200
H	-0.28902200	2.21959800	-2.42916900
H	0.74142000	3.53579100	-3.06924100
H	-0.84827600	3.90212200	-2.33672700
H	1.38627000	0.55543300	1.28344000
H	3.65731600	0.85742100	2.29181900
H	5.69173100	0.66017300	0.82814700
H	5.43947300	0.20148100	-1.59741600
H	0.79255400	0.16525300	-2.37270100
C	4.17566600	-0.46868600	-3.65333000
H	4.82613700	0.42177000	-3.76238600
H	4.76862400	-1.30714600	-3.24074800

H	3.77554500	-0.75040100	-4.63879300
C	1.21383400	-2.50206400	0.18302900
C	0.71690600	-2.04624300	1.44023900
S	-0.61929000	-0.89124900	1.57575000
S	0.42595300	-2.01687300	-1.34896800
C	2.38247100	-3.28839100	0.13712300
C	1.40167400	-2.47823300	2.60418300
C	3.04402600	-3.69364400	1.30256800
H	3.94809600	-4.30340800	1.23639700
C	2.53615600	-3.29085200	2.54471200
H	3.03476100	-3.59029300	3.47089500
Cl	0.84358200	-1.94840400	4.18824800
Cl	3.08011800	-3.77548900	-1.40738900

Cat._L3

E(BP86)= -2505.4749157 Hartree

Ru	-0.18236200	-0.40239900	0.37089700
S	-1.20921000	0.94892400	1.98449700
S	-1.90929500	-2.06043300	0.56350500
O	1.00620700	-1.86901100	-0.94816200
O	-4.74289000	1.21826200	3.11135200
O	-5.42732800	-1.76442900	1.72278000
N	-0.74203800	1.85530900	-1.36680300
N	1.40466500	1.94604500	-0.86390700
C	-1.99271900	1.17000500	-1.56967400
C	-3.13273100	1.54843200	-0.82382700
C	-4.27298200	0.73210200	-0.91489400
C	-4.31231700	-0.40998900	-1.73448800
C	-3.19762100	-0.68533600	-2.54850100
C	-2.03125800	0.09038600	-2.48755100
C	-3.16109800	2.80160100	0.01782600
C	-5.51555700	-1.32231100	-1.71455800
C	-0.84999100	-0.21325100	-3.38207400
C	-0.25269200	2.97101800	-2.20153600
C	1.17555200	3.18276500	-1.64933800
C	0.26116800	1.23892600	-0.67739500
C	2.68656500	1.62640100	-0.31506100
C	3.02996000	2.07961300	0.97507000
C	4.29996000	1.73600500	1.47404200
C	5.21133700	0.97398500	0.72348700
C	4.83234700	0.54630000	-0.56296500
C	3.57578900	0.85799000	-1.09972700
C	2.05331100	2.88095700	1.80100900
C	6.56237800	0.59461000	1.28454500

C	3.16426900	0.35793900	-2.46445200
C	2.22013300	-2.16232600	-0.33171800
C	2.41452700	-1.48977200	0.90180800
C	3.61973300	-1.73375700	1.59966400
C	4.58857200	-2.59894100	1.07600100
C	4.36786100	-3.23946000	-0.15506900
C	3.17068800	-3.03302200	-0.86681000
C	1.36188600	-0.61524800	1.38284200
C	-2.68697800	0.09177200	2.15149900
C	-2.97716800	-1.14975400	1.56294700
C	-4.42646300	-1.09969000	1.94773300
C	-4.10596800	0.30739100	2.60628300
H	-5.14611500	0.98143200	-0.30005200
H	-3.22999900	-1.54458000	-3.22974700
H	-2.14754600	3.12562300	0.29690300
H	-3.73300700	2.64408300	0.94713100
H	-3.65307200	3.62144700	-0.54185600
H	-5.45439200	-2.09208300	-2.50231500
H	-6.45402600	-0.75603800	-1.85434700
H	-5.58754200	-1.82980100	-0.73465400
H	-0.67845300	0.59455200	-4.11864800
H	-1.02137500	-1.14115800	-3.95258300
H	0.08359200	-0.32917700	-2.80456600
H	-0.89741900	3.85681800	-2.08031700
H	-0.25048900	2.68081700	-3.26967000
H	1.93660700	3.28458100	-2.44085400
H	1.24312700	4.06637800	-0.98722900
H	4.58105400	2.07343000	2.47926200
H	5.52294200	-0.06913600	-1.15150900
H	1.71764900	3.79293500	1.27459800
H	2.50795800	3.19244500	2.75560800
H	1.14563700	2.29450500	2.03001800
H	7.38482700	0.96824000	0.64735900
H	6.66791400	-0.50485500	1.33698800
H	6.70956800	0.99973500	2.29976800
H	2.26737900	-0.28121000	-2.39348300
H	3.97297700	-0.23455300	-2.92264600
H	2.91628600	1.18618900	-3.15397200
H	3.77901900	-1.22872800	2.55785700
H	5.51329000	-2.78599000	1.63170000
H	5.12281100	-3.91758900	-0.56626100
H	2.99776300	-3.54466800	-1.81749100
H	1.48356300	-0.20508400	2.39985500
C	0.40987600	-2.90920100	-1.76056000

H	0.94389900	-2.99158400	-2.72267000
H	0.43593500	-3.86669600	-1.21497200
H	-0.62889100	-2.59550300	-1.92483300

TS1_L2

E(BP86)= -2505.43511213 Hartree

Ru	0.18906300	-0.26302000	-0.60724300
O	-1.44495400	-1.38956800	1.67503300
N	0.71858700	2.36951100	0.71789200
N	-1.45933500	2.13970900	0.49382400
C	2.10345100	1.98570000	0.70592900
C	2.86414500	2.25693800	-0.45103700
C	4.16844700	1.74079300	-0.51680200
C	4.71791000	0.97653800	0.52912500
C	3.93836300	0.75949100	1.68071600
C	2.63026700	1.25515000	1.79312500
C	2.26457100	3.01127800	-1.61274600
C	6.10957800	0.39582800	0.41884600
C	1.78839900	0.96612500	3.01224800
C	0.18786300	3.56563100	1.40755600
C	-1.30890000	3.51725200	1.02934200
C	-0.25821800	1.54237800	0.27060500
C	-2.71349200	1.67345700	-0.01808300
C	-2.96237200	1.75254500	-1.40637500
C	-4.17664300	1.23637500	-1.88838900
C	-5.13140100	0.66114100	-1.03075100
C	-4.85889200	0.62737300	0.34785300
C	-3.66055100	1.13162900	0.87673400
C	-1.93279100	2.32830800	-2.34806500
C	-6.41106900	0.06586000	-1.57088100
C	-3.38471700	1.07702900	2.35962900
C	-2.48384000	-1.94632300	0.98591000
C	-2.45508900	-1.77470300	-0.43519800
C	-3.53156800	-2.32122400	-1.18122000
C	-4.58790900	-3.00126400	-0.56811900
C	-4.59344400	-3.14991600	0.82827500
C	-3.54624700	-2.62439600	1.60432200
C	-1.45071700	-0.99412000	-1.11068000
H	4.75802300	1.90686400	-1.42601400
H	4.34398500	0.14468500	2.49265900
H	1.55935700	2.36549700	-2.16775100
H	3.04860200	3.33290200	-2.31760500
H	1.70406200	3.90408800	-1.28290400
H	6.86724900	1.10219500	0.80946300

H	6.36669600	0.16982100	-0.62905700
H	6.19556400	-0.54211400	0.99227200
H	1.71235600	1.84785900	3.67817600
H	2.22459500	0.14112300	3.59813100
H	0.76408100	0.67479700	2.72066600
H	0.69821700	4.47670100	1.05407500
H	0.35020900	3.47518200	2.49822100
H	-1.97988200	3.67395000	1.88954600
H	-1.57268300	4.25108200	0.24406900
H	-4.37694700	1.27523000	-2.96630200
H	-5.58350500	0.16464300	1.02827900
H	-1.56574500	3.31486600	-2.01255400
H	-2.34609700	2.44278200	-3.36365000
H	-1.04311600	1.66999000	-2.41282300
H	-7.30164100	0.52333100	-1.10257400
H	-6.44854000	-1.01797300	-1.35714100
H	-6.49276700	0.20164200	-2.66242600
H	-2.31170900	0.91709000	2.55128000
H	-3.95295500	0.25579600	2.82767800
H	-3.68466100	2.01507600	2.86581400
H	-3.51815000	-2.18798600	-2.26858000
H	-5.39546900	-3.42460600	-1.17432800
H	-5.40952000	-3.68622700	1.32433800
H	-3.56315800	-2.75025400	2.69000600
H	-1.62161800	-0.84597200	-2.19691800
C	-1.28809800	-1.73315700	3.05416500
H	-2.10595700	-1.31690700	3.67244600
H	-1.24270300	-2.82970800	3.18136900
H	-0.32958200	-1.28865800	3.35715300
S	1.35916400	-1.65683500	0.79947000
S	1.82650400	-0.55191200	-2.19875000
C	4.42794700	-2.00106700	-1.44118700
O	5.37052900	-1.90340500	-2.20753900
C	4.19727600	-2.52472500	0.04787100
O	4.88429500	-2.99845300	0.93643400
C	2.99423600	-1.55376100	-1.39938700
C	2.78854500	-2.01500900	-0.09687000

2_L2

E(BP86)= -2505.44840356 Hartree

Ru	0.21455600	-0.16884600	-0.77649600
S	1.97404400	-1.22060300	-2.08619000
S	0.77849800	-1.35000800	1.12268900
O	-2.04856000	-2.17469200	0.95746600

N	1.16195800	2.11975000	0.73777000
N	-1.04392800	2.24089400	0.63227400
C	2.49077700	1.74519000	0.33048600
C	2.91165800	2.03818100	-0.98942300
C	4.19567400	1.63155000	-1.37924700
C	5.05968200	0.95194700	-0.50137000
C	4.62321500	0.71729600	0.81446700
C	3.34844300	1.10982200	1.25785000
C	1.99214300	2.70479900	-1.98385500
C	6.40218700	0.44526700	-0.97274000
C	2.93476400	0.85180400	2.68725900
C	0.87036900	3.43362700	1.34620200
C	-0.66990700	3.41217900	1.46027600
C	0.04260800	1.49513700	0.27591800
C	-2.40549300	1.80249200	0.56318900
C	-3.20520100	2.24717800	-0.51083600
C	-4.54007000	1.81383700	-0.56681100
C	-5.08227400	0.96315800	0.41300300
C	-4.25607800	0.55331600	1.47596700
C	-2.91723500	0.96092600	1.57677600
C	-2.62203700	3.14345600	-1.57833900
C	-6.50486700	0.46622600	0.31216200
C	-2.04338100	0.50323500	2.71800100
C	-3.00151300	-2.11180400	-0.00120400
C	-2.74442700	-1.20992800	-1.08229200
C	-3.74143100	-1.08759600	-2.08547500
C	-4.91896600	-1.83766900	-2.06065300
C	-5.13768500	-2.73044700	-0.99764300
C	-4.19298100	-2.86058100	0.03139100
C	-1.56405100	-0.39041700	-1.19609300
H	4.52249300	1.82728900	-2.40750700
H	5.28049400	0.18588700	1.51290700
H	1.29184000	1.95905800	-2.41331300
H	2.56636200	3.14087400	-2.81812000
H	1.37651300	3.50118900	-1.53065900
H	7.16795900	0.53084700	-0.18217700
H	6.75343800	0.99683000	-1.86153600
H	6.32432900	-0.62457100	-1.24127300
H	3.41270500	1.58009000	3.37093700
H	3.24985100	-0.15738000	3.00423300
H	1.84324500	0.92067400	2.81039000
H	1.23476400	4.24315600	0.68515000
H	1.37666200	3.52819200	2.32135400
H	-1.01325500	3.26189800	2.50053800

H	-1.14510800	4.32847600	1.07083800
H	-5.17084700	2.14197700	-1.40194600
H	-4.66505400	-0.11131600	2.24695500
H	-2.33712000	4.13281900	-1.17384800
H	-3.34714200	3.31124800	-2.39178700
H	-1.70577800	2.70615000	-2.01495500
H	-6.98246000	0.40004300	1.30544600
H	-6.52284800	-0.54560500	-0.13327200
H	-7.12105600	1.12345200	-0.32476400
H	-1.11627700	0.03413500	2.34902800
H	-2.57299500	-0.23411200	3.34286100
H	-1.74924900	1.34298300	3.37601500
H	-3.55669200	-0.38228100	-2.90367000
H	-5.66016300	-1.72958700	-2.85852600
H	-6.05326700	-3.33105400	-0.96059500
H	-4.38626800	-3.55032400	0.85638800
H	-1.65568500	0.36482500	-2.03236500
C	-2.22219300	-3.09071500	2.03878600
H	-3.11175000	-2.83141000	2.64487500
H	-2.31284600	-4.12993200	1.67229900
H	-1.31082900	-2.99233400	2.64525000
C	2.76747200	-1.91504800	-0.72706500
C	2.29399600	-1.94940900	0.59942400
C	4.11496200	-2.46178400	-0.34654000
O	5.17120700	-2.69826500	-0.90873500
C	3.59408300	-2.45953700	1.15417200
O	4.07176200	-2.65476700	2.26025800

3_L2

E(BP86)= -2505.43281827 Hartree

Ru	0.57165500	-0.09402000	-0.50919800
O	-1.58830300	2.58925300	-2.35150800
N	1.91797000	-2.55591400	0.10554800
N	-0.23560600	-3.02057000	0.18453700
C	3.03800800	-1.65638300	0.04345100
C	3.56233200	-1.09921600	1.23247500
C	4.54302100	-0.10119900	1.11309800
C	4.99788200	0.35059400	-0.13811800
C	4.47514500	-0.24648100	-1.29847500
C	3.48760700	-1.24167600	-1.23432500
C	3.06865800	-1.53894600	2.58959300
C	5.98418600	1.49117400	-0.23702800
C	2.87792600	-1.80254700	-2.49992200
C	1.89981600	-3.95114100	0.58550000

C	0.42453100	-4.34171200	0.32599500
C	0.66701700	-2.03066900	-0.03071600
C	-1.65323200	-2.85673800	0.07876800
C	-2.40250700	-2.71452100	1.26571100
C	-3.78599300	-2.49704300	1.15028700
C	-4.41346300	-2.37437500	-0.10260700
C	-3.63451600	-2.53946400	-1.26202300
C	-2.25468700	-2.79526900	-1.19678300
C	-1.71987100	-2.70398700	2.61300400
C	-5.87592900	-2.00555000	-0.19724900
C	-1.43792100	-2.99740600	-2.45174300
C	-2.29985100	2.37600600	-1.20443300
C	-2.13180100	1.09070300	-0.60856200
C	-2.83244000	0.80162200	0.57902600
C	-3.67715400	1.74680600	1.16963000
C	-3.79845300	3.02315700	0.59571100
C	-3.11192900	3.34355900	-0.58432000
C	-1.11289500	0.20880500	-1.17840900
H	4.93846900	0.35922400	2.02633100
H	4.81796000	0.09702000	-2.28182200
H	1.97444200	-1.67798500	2.59362900
H	3.30755200	-0.78206100	3.35369500
H	3.53674400	-2.49212000	2.90408600
H	6.64342700	1.38399900	-1.11584900
H	6.61584600	1.56347700	0.66465900
H	5.44572300	2.45154300	-0.34406800
H	2.63159400	-2.87337600	-2.40232900
H	3.55829000	-1.66876500	-3.35729400
H	1.93236200	-1.27770000	-2.74894000
H	2.15943100	-3.99954100	1.66013300
H	2.61540300	-4.57196500	0.02198100
H	0.30413400	-4.92379300	-0.60802700
H	-0.02415400	-4.91419000	1.15367200
H	-4.37993100	-2.36913300	2.06359400
H	-4.11129400	-2.45610900	-2.24627400
H	-1.06060300	-3.57818800	2.76107700
H	-2.46100800	-2.69565700	3.42895800
H	-1.09134800	-1.79952900	2.71647000
H	-6.32253400	-2.34376900	-1.14776000
H	-5.99286300	-0.90616400	-0.14765300
H	-6.46013600	-2.43661600	0.63415000
H	-0.52702600	-2.37383100	-2.44554100
H	-2.02513800	-2.73949900	-3.34841600
H	-1.11206900	-4.04970200	-2.55807800

H	-2.67902100	-0.17478300	1.03919600
H	-4.20552800	1.50385400	2.09688200
H	-4.41976100	3.78639700	1.07607300
H	-3.19593900	4.34680900	-1.00936500
H	-1.19801200	-0.02864500	-2.26514800
C	-1.33145000	3.95129800	-2.72252700
H	-2.25212700	4.45738600	-3.07243800
H	-0.88583300	4.50945900	-1.87907000
H	-0.60845200	3.89606300	-3.54886200
C	0.77835500	2.82410500	0.34170100
C	0.28794400	2.18108900	1.49500700
S	0.21971400	0.48260800	1.71066100
S	1.50592800	2.09301700	-1.04111500
C	-0.18775100	3.46640100	2.13060800
O	-0.74863900	3.80108000	3.15677600
C	0.32732900	4.17772800	0.80260600
O	0.26747700	5.29814300	0.32025300

TS2_L3

E(BP86)= -2505.41488022 Hartree

Ru	-0.92276100	-0.25646600	-0.51109200
O	2.92549200	-2.13188600	-2.18891600
N	-2.82916100	1.79453600	-0.22014700
N	-0.89558400	2.84644300	-0.10878500
C	-3.58726700	0.57786900	-0.21646000
C	-4.35270800	0.18214300	0.90430400
C	-4.91969200	-1.10233300	0.90342100
C	-4.69453500	-2.02333900	-0.14011100
C	-3.91191600	-1.61999300	-1.22936600
C	-3.34452900	-0.32603700	-1.30177700
C	-4.47715200	1.06988000	2.12018300
C	-5.24270700	-3.43002300	-0.05613300
C	-2.59690000	0.10902800	-2.54710700
C	-3.24665300	3.19012900	0.00114700
C	-1.89525500	3.94022900	-0.14822900
C	-1.46619100	1.62436100	-0.23796600
C	0.51448200	3.08900600	-0.06705800
C	1.11698700	3.33801000	1.18501600
C	2.50542100	3.55216400	1.21757500
C	3.29155700	3.48523200	0.05352600
C	2.65183100	3.24310300	-1.17513700
C	1.26419500	3.04988300	-1.26157900
C	0.30650400	3.27848100	2.45857700
C	4.79629300	3.59319100	0.12895000

C	0.59361000	2.76874100	-2.58456900
C	3.24789800	-1.39804300	-1.08323800
C	2.22239400	-0.53837800	-0.58135900
C	2.51570300	0.24330200	0.55180700
C	3.76363800	0.18871700	1.18261400
C	4.74190100	-0.69368500	0.70106800
C	4.48666400	-1.49109500	-0.42468500
C	0.89250700	-0.52277400	-1.21878600
H	-5.50893800	-1.41432500	1.77420100
H	-3.72027400	-2.32114600	-2.04968600
H	-3.48209600	1.43155100	2.43835900
H	-4.91624600	0.51175600	2.96281900
H	-5.11627300	1.95519100	1.94059200
H	-5.29755800	-3.90340700	-1.05110500
H	-6.25215900	-3.44619900	0.39084000
H	-4.59341600	-4.06484000	0.57593700
H	-2.83843900	1.14907400	-2.82672200
H	-2.81564800	-0.56845600	-3.38846400
H	-1.45869700	0.11085100	-2.47640900
H	-3.68183800	3.32589300	1.00717500
H	-3.99388400	3.50654100	-0.74642000
H	-1.81936600	4.48033500	-1.11113500
H	-1.71637200	4.66296100	0.66492900
H	2.99076700	3.73052800	2.18495600
H	3.25258300	3.18495000	-2.09093000
H	-0.53857400	3.99152600	2.45991800
H	0.93667700	3.50423000	3.33429200
H	-0.11719700	2.26624700	2.59641400
H	5.22100800	4.03989300	-0.78661900
H	5.23754000	2.58430900	0.24224700
H	5.12024600	4.19763300	0.99359200
H	0.17104900	1.74808200	-2.58676000
H	1.31202200	2.85015000	-3.41654400
H	-0.24087000	3.46670400	-2.78243100
H	1.73149100	0.89487100	0.93289400
H	3.95391700	0.80877300	2.06411900
H	5.70928900	-0.77848300	1.20841300
H	5.24939800	-2.18710800	-0.78255600
H	0.97117800	-0.49205600	-2.32405800
C	3.62561500	-3.37009200	-2.38129200
H	4.68141000	-3.20478700	-2.67044800
H	3.56700700	-3.98619000	-1.46570700
H	3.10153100	-3.87580600	-3.20571900
C	0.68091700	-2.82099100	0.53090100

C	0.48859900	-2.00098600	1.65656800
S	-0.37819500	-0.52583600	1.73069600
S	0.04805100	-2.56195300	-1.06334700
C	1.45423900	-2.82454800	2.50139600
O	1.88921800	-2.77571300	3.63471800
C	1.69407300	-3.69383500	1.18992000
O	2.45286400	-4.58750800	0.84298400

4_L3

E(BP86)= -2505.41622041 Hartree

Ru	-0.95286200	-0.25849900	-0.50639000
O	3.03835600	-2.21986300	-2.08989500
N	-2.81232500	1.81256900	-0.18384000
N	-0.87025700	2.84357100	-0.05672100
C	-3.58410000	0.60467800	-0.20923400
C	-4.36457000	0.19683500	0.89800000
C	-4.96475800	-1.07094800	0.85889000
C	-4.76246800	-1.96657900	-0.21262700
C	-3.96305200	-1.55497200	-1.28548000
C	-3.35926700	-0.27492100	-1.31861000
C	-4.47437800	1.05739000	2.13470400
C	-5.36336500	-3.35376900	-0.17558700
C	-2.60117800	0.17950300	-2.55058000
C	-3.21844200	3.20751600	0.05518100
C	-1.86092400	3.94580600	-0.08971400
C	-1.44985500	1.62532500	-0.20475800
C	0.53908600	3.08964800	-0.04038900
C	1.16092500	3.34945200	1.20007400
C	2.54713600	3.57827700	1.20843000
C	3.31383200	3.51423700	0.03136100
C	2.65597100	3.25902100	-1.18485500
C	1.26925100	3.05137800	-1.24693300
C	0.37214100	3.28310300	2.48701900
C	4.81857800	3.63494600	0.08065300
C	0.57956100	2.75548200	-2.55643700
C	3.31247000	-1.42465400	-1.00763900
C	2.25107700	-0.58035800	-0.57038400
C	2.49468600	0.26992800	0.51753400
C	3.73182400	0.29055100	1.17698200
C	4.75220000	-0.57320200	0.75754700
C	4.54581600	-1.43349700	-0.33213500
C	0.90941600	-0.65291300	-1.23134600
H	-5.56577200	-1.39218800	1.71829600
H	-3.79103300	-2.23563400	-2.12737900

H	-3.47396200	1.39672500	2.46039900
H	-4.92264300	0.48707000	2.96429300
H	-5.09934600	1.95666400	1.97558400
H	-5.31247000	-3.84311100	-1.16287100
H	-6.42107700	-3.32898400	0.14197800
H	-4.82204800	-3.99784300	0.54270700
H	-2.83064900	1.22800600	-2.80829100
H	-2.82259400	-0.47668500	-3.40783900
H	-1.46269400	0.16978400	-2.47520500
H	-3.64866900	3.33498100	1.06478300
H	-3.96570000	3.54046700	-0.68537700
H	-1.77998700	4.49053300	-1.04980100
H	-1.67548000	4.66279500	0.72712300
H	3.04729500	3.76586500	2.16650500
H	3.24216200	3.20095000	-2.11006800
H	-0.47144100	3.99776300	2.50789900
H	1.01748900	3.50169900	3.35347900
H	-0.05317100	2.27163700	2.62521700
H	5.22364800	4.08585700	-0.84175700
H	5.26911600	2.62918000	0.18512100
H	5.15272800	4.24116400	0.94019200
H	0.15534700	1.73567200	-2.53787900
H	1.28558400	2.82625700	-3.39990700
H	-0.25757100	3.45158400	-2.75044600
H	1.67807600	0.90650300	0.85470000
H	3.87954200	0.95966700	2.03055500
H	5.71379900	-0.59394800	1.28252000
H	5.34242100	-2.11134300	-0.64925900
H	0.99203200	-0.45558800	-2.31979900
C	3.80187200	-3.42603600	-2.22741000
H	4.85518700	-3.21824600	-2.49800100
H	3.75122800	-4.01967600	-1.29674000
H	3.32414600	-3.98158800	-3.04828500
C	0.70761800	-2.82920500	0.46542600
C	0.44469300	-2.06303100	1.61428600
S	-0.41269900	-0.59627000	1.72076300
S	0.17793700	-2.45030300	-1.16339900
C	1.32622800	-2.97180200	2.47704700
O	1.67120400	-3.00551900	3.63883400
C	1.63512600	-3.77613200	1.13218200
O	2.37641100	-4.68789200	0.79701500