

Electronic supplementary information

A theoretical elucidation: why do a SO₃H-functionalized imidazolium-based ionic liquid catalyzes the conversion of 5-hydroxymethylfurfural to levulinic acid?

Jingjing Li,^{a,b} Yaru Jing,^a Chengbu Liu,^a and Dongju Zhang^{*a}

^aKey Lab of Colloid and Interface Chemistry, Ministry of Education, Institute of Theoretical Chemistry, Shandong University, Jinan, 250100, P. R. China

^bCollege of Arts and Sciences, Shanxi Agricultural University, Taigu Shanxi, 030801, P. R. China

*Corresponding Author: zhangdj@sdu.edu.cn.

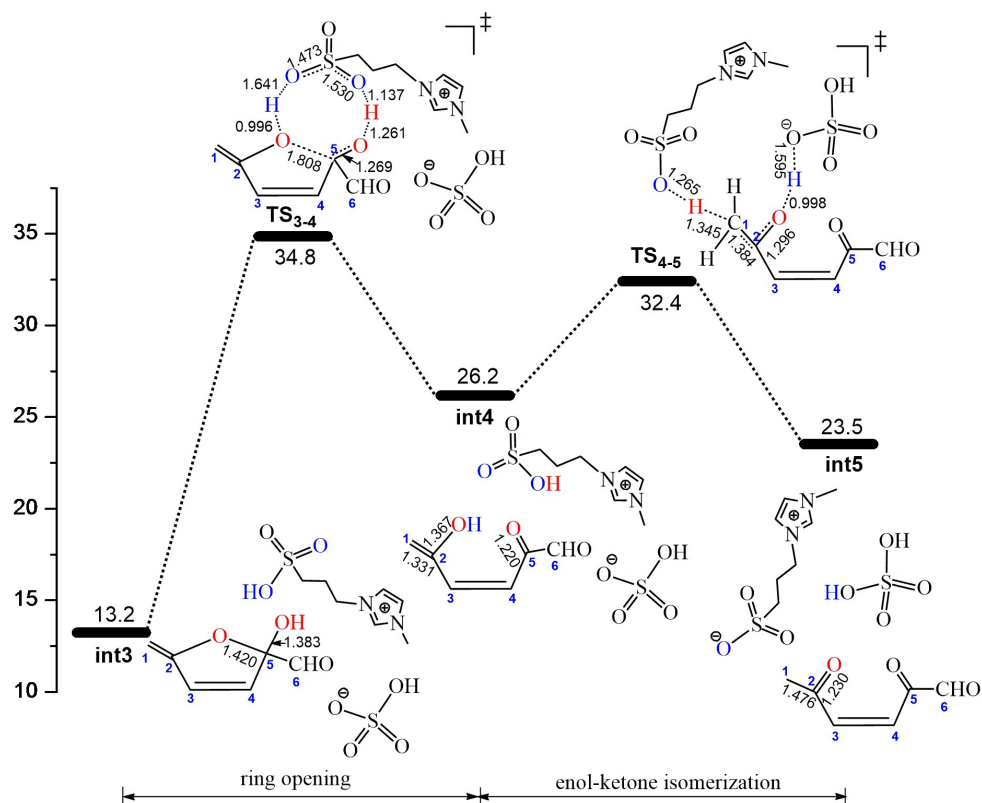


Fig. S1 Calculated Gibbs free energy profile with schematic geometries for the furan ring opening and the first enol-ketone isomerization processes.

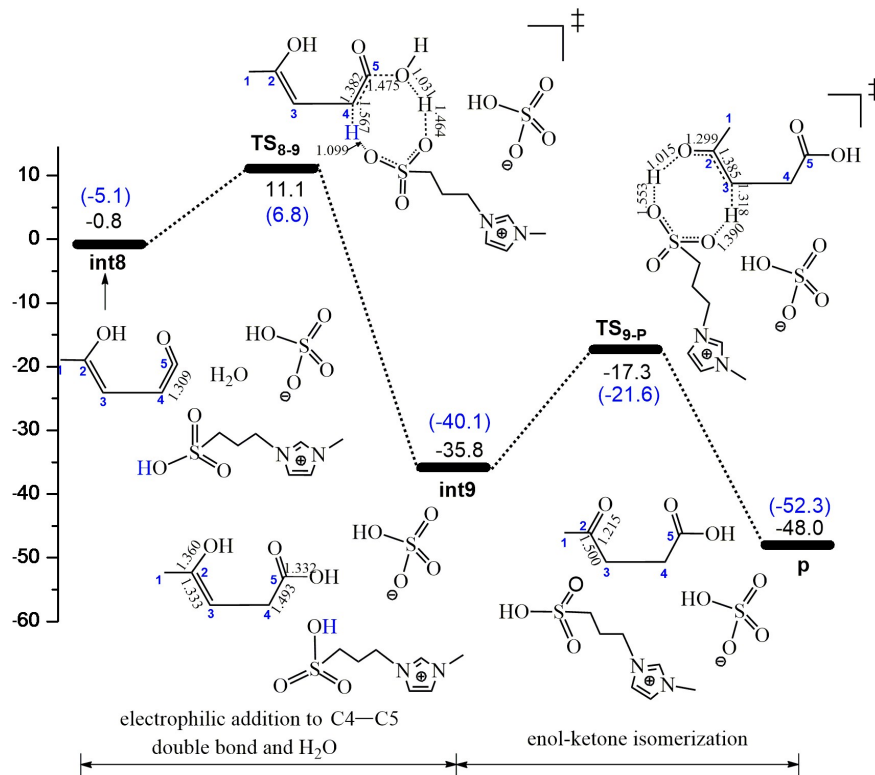


Fig. S2 Calculated Gibbs free energy profile with schematic geometries for the addition of H₂O molecule on the C4-C5 double bond and the second enol-ketone isomerization.

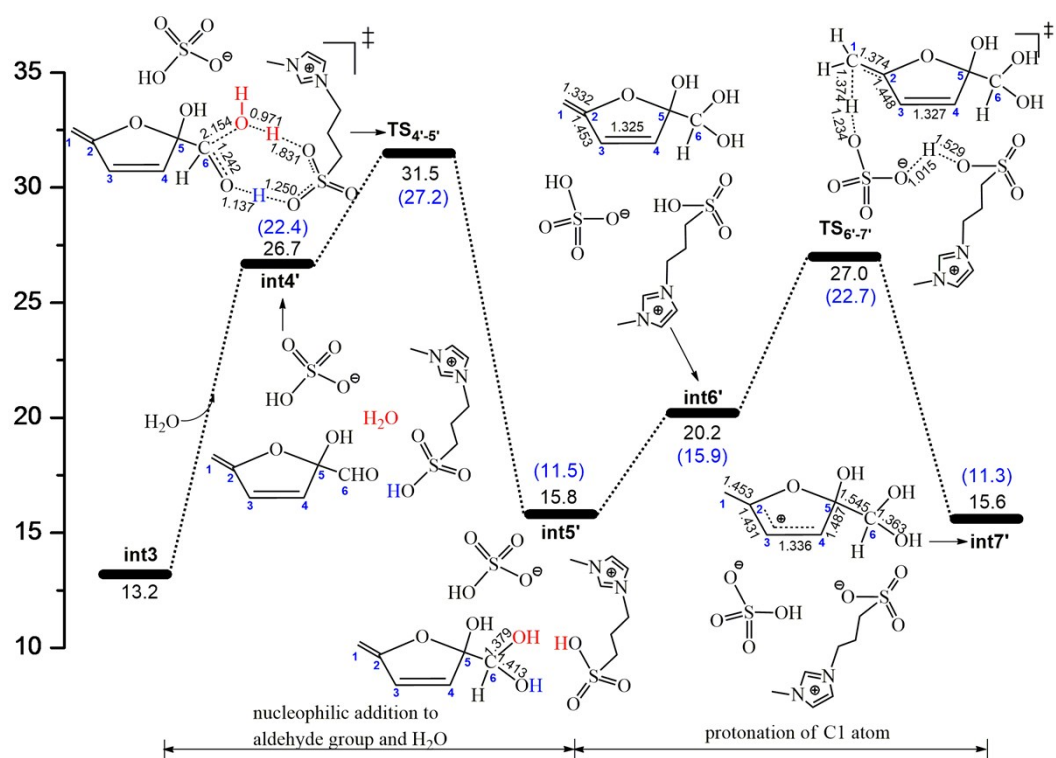


Fig. S3 Calculated Gibbs free energy profile with schematic geometries for the addition of H₂O to the aldehyde group resulting in the gem-diol group intermediate.

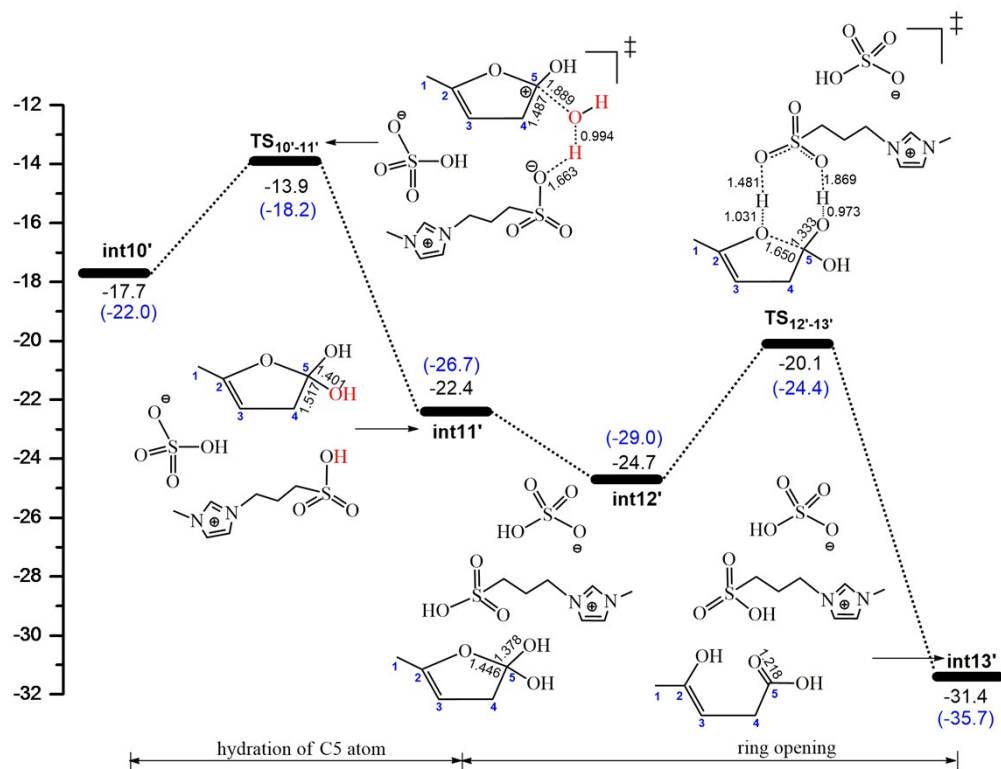


Fig. S4 Calculated Gibbs free energy profile with schematic geometries for the conversion of **int10'** to **int13'**.

Cartesian Coordinates of All the Structures

int1

O	-1.17160300	-4.05351500	0.20815800
H	-0.39679600	-3.17154400	-0.83349100
C	2.33878900	1.19932000	1.04570900
C	4.00366600	-0.12975600	0.54086300
N	3.11479800	0.79237300	0.05445600
H	1.54554200	1.91917600	0.95769400
H	4.73730800	-0.60113500	-0.08413100
C	3.01170600	1.24804500	-1.32332800
C	2.71432300	0.13047200	-2.29559600
H	3.94982400	1.72588900	-1.58774200
H	2.22855300	1.99899900	-1.34362800
C	1.36585400	-0.54315400	-2.12206600
H	3.50999000	-0.61227100	-2.28870800
H	2.72217400	0.57625000	-3.28692800
H	0.59193600	0.14099000	-1.78165900
H	1.04716000	-0.98195600	-3.06355800
S	1.36274200	-1.91411000	-0.99675500
O	0.11656700	-2.68434800	-1.55410900
O	2.56351900	-2.70104500	-1.21312000
O	1.08390600	-1.50982200	0.37042800
H	-1.84702800	-4.55773600	-0.25302900
C	-2.70359600	-2.34326900	0.94511200
C	-3.93952500	-1.99898700	1.39957700
H	-4.51169500	-2.52836500	2.13901300
C	-4.29647200	-0.81976400	0.71591300
C	-2.98598700	0.51153000	-1.05585100
H	-2.06674000	0.38378800	-1.63452600
C	-3.25993100	-0.53761500	-0.12167600
O	-2.28576700	-1.47353900	0.02007800
O	-3.70388800	1.49056200	-1.20743900
C	-1.75311700	-3.41198600	1.32862000
H	-2.25996200	-4.13217000	1.96426600
H	-5.20158300	-0.24782600	0.81239900
H	-0.92595300	-2.98460900	1.88965400
S	-0.98025100	3.21030100	0.01781300
O	-0.83399200	1.77421300	0.27494700
O	-1.60398800	3.33259000	-1.46039400
O	0.29159700	3.91233200	-0.12417400
O	-1.93086900	3.85786200	0.91936700
H	-2.43933300	2.83089400	-1.49493100
N	2.71346700	0.58653000	2.15465200

C	2.10748300	0.75086400	3.46052000
H	1.63035400	-0.17619700	3.75789000
H	2.87458000	1.01687300	4.17842400
H	1.36941900	1.54106700	3.40657600
C	3.74818300	-0.25981800	1.85972700
H	4.21241400	-0.86909500	2.61066200

TS₁₋₂ (imaginary frequency = -59.59 cm⁻¹)

O	2.94623000	3.31812100	-0.27344700
H	3.60213800	2.61002700	-0.41037400
C	1.59518300	-3.02302300	0.41831300
C	1.14245000	-3.32125700	-0.81913500
C	0.08870900	-1.53697600	-0.12590300
N	0.91526800	-1.91000700	0.83370300
H	2.32701100	-3.50886000	1.03366500
H	1.39811400	-4.11468100	-1.49325700
H	-0.58246300	-0.69737500	-0.08946800
N	0.19774600	-2.38048400	-1.13644100
C	1.09878500	-1.21259700	2.09861800
C	2.51782000	-0.75040100	2.33756500
H	0.79332300	-1.88431100	2.89498100
H	0.41611000	-0.36688700	2.08846200
C	3.02959900	0.36150300	1.44210500
H	3.20745800	-1.59263200	2.31484400
H	2.53225800	-0.37530900	3.36020300
H	2.24916000	1.07897900	1.18746400
H	3.81639400	0.90332900	1.95908900
C	-0.56460900	-2.32468900	-2.36436700
H	0.11618900	-2.28629100	-3.20897700
H	-1.19622800	-3.20186500	-2.44442900
H	-1.17987600	-1.43401400	-2.35413200
S	3.79500500	-0.13807500	-0.09095400
O	4.62195500	1.03178800	-0.47118100
O	4.59789700	-1.33297300	0.20567900
O	2.72948300	-0.39033700	-1.07991500
H	3.15321400	3.96252800	-0.95932900
C	-0.08440200	2.64572900	-0.94431200
C	-0.97617800	3.70664500	-1.18036600
H	-0.82409000	4.47792900	-1.91483400
C	-2.03750200	3.54772600	-0.32243200
C	-2.52233300	1.74293500	1.47767200
H	-2.05711900	0.86431600	1.92596700
C	-1.74736100	2.40530200	0.40298700
O	-0.60509500	1.86660600	0.06221900

O	-3.57539500	2.20395200	1.83113000
C	1.08073400	2.31221500	-1.52723800
H	1.44306800	2.92388300	-2.33757800
H	-2.91694000	4.15459600	-0.21154200
H	1.61572400	1.40785700	-1.27020600
S	-3.78861900	-1.08921500	-0.19512400
O	-2.92043100	0.05272000	-0.50920500
O	-4.32933100	-0.81894900	1.30404700
O	-3.07992900	-2.34951200	-0.02983900
O	-4.97196800	-1.15281000	-1.04694000
H	-4.83942000	0.00135100	1.32443900
int2			
C	2.39713600	2.10475700	1.33543300
C	2.98058000	2.84513200	0.23794800
H	3.38628100	3.83652700	0.34188700
C	2.93828900	2.10334200	-0.86079300
C	1.11215800	0.45366300	-1.33514600
H	0.29124200	1.16468900	-1.21536800
C	2.33348600	0.78659000	-0.49969000
O	1.95149800	0.89434200	0.82649300
O	1.06264000	-0.47904300	-2.09466000
C	2.24796000	2.41834700	2.61076100
H	2.57782100	3.38234700	2.95988500
O	-0.35435600	3.45580200	-0.06789400
H	-0.95851300	3.24957200	-0.79292400
H	3.28818900	2.32672000	-1.85280200
H	1.80363700	1.72862000	3.30963200
C	-3.53659200	-1.34039100	1.56640400
C	-2.84312400	-0.85409200	2.61755000
C	-1.41089400	-1.67028900	1.18601600
N	-2.62079700	-1.85929500	0.69125600
H	-4.59141100	-1.37390100	1.37420600
H	-3.17259300	-0.37365300	3.51817000
H	-0.49075500	-1.94758400	0.70832300
N	-1.51772000	-1.08577000	2.36524600
C	-2.91287600	-2.41931000	-0.61872400
C	-3.56935500	-1.42586900	-1.55109500
H	-3.56521300	-3.27518600	-0.47560600
H	-1.97134700	-2.77504100	-1.02468500
C	-2.72260400	-0.24720500	-1.99066600
H	-4.50348900	-1.06859000	-1.12117700
H	-3.83938700	-1.98662400	-2.44351500
H	-1.67934300	-0.51699200	-2.14420100

H	-3.10513800	0.13384300	-2.93377100
C	-0.40632700	-0.59048400	3.15188000
H	-0.33638000	0.48571900	3.03671100
H	-0.56613400	-0.83740500	4.19476900
H	0.50474200	-1.05894100	2.80216100
S	-2.73480700	1.18479700	-0.92562500
O	-2.26114000	2.28173700	-1.80255400
O	-4.12390100	1.36236900	-0.47509300
O	-1.79470200	0.94888600	0.18641500
S	3.15512700	-1.73359300	-0.35105600
O	1.92708100	-1.89832200	0.37407700
O	3.04317500	-2.34340700	-1.78445800
O	4.38633400	-2.21495700	0.19196500
O	3.37508900	-0.19076400	-0.67257800
H	-0.47579200	2.68151200	0.48602500
H	2.30729900	-1.89773500	-2.24931800

TS_{2,3} (imaginary frequency = -246.11cm⁻¹)

C	-2.42750800	-2.15917200	1.80053000
C	-3.48622900	-2.48261200	0.88552400
H	-4.41440600	-2.93546600	1.18698000
C	-3.10120400	-2.12458100	-0.34788900
C	-1.10723100	-0.62341400	-1.12609800
H	-0.29328800	-0.05147900	-0.67966000
C	-1.77580500	-1.59634800	-0.20505500
O	-1.41927800	-1.54867300	1.05306800
O	-1.46086200	-0.53149800	-2.27200700
C	-2.28810000	-2.34175600	3.10347400
H	-3.09220500	-2.79713800	3.65759600
O	-0.71289400	-3.07764400	-0.92814600
H	0.15989600	-2.75663800	-1.28115700
H	-3.62175400	-2.20812500	-1.28326200
H	-1.38840900	-2.04895500	3.61943000
C	3.10818000	1.09371100	2.15876400
C	2.08375900	0.81230800	2.99141300
C	1.25269900	1.72081500	1.18330700
N	2.56748100	1.67079000	1.04163100
H	4.16446400	0.93850800	2.26402100
H	2.06961100	0.37369500	3.97003100
H	0.55513700	2.12315100	0.46694700
N	0.93610100	1.21591800	2.36373300
C	3.30841100	2.10121700	-0.13444400
C	3.80486500	0.95084500	-0.98259100
H	4.14613900	2.69541600	0.21595900

H	2.64972700	2.74876700	-0.70417300
C	2.70712200	0.16065300	-1.68380600
H	4.43492400	0.29498000	-0.38337700
H	4.45595600	1.38638200	-1.73593800
H	1.74226800	0.66548400	-1.64408900
H	2.94749600	0.00879600	-2.73224900
C	-0.39966500	1.15834900	2.92216600
H	-0.55677000	0.18260900	3.36522600
H	-0.51016700	1.92485500	3.68180500
H	-1.11690900	1.31999800	2.12733500
S	2.46216100	-1.47117600	-1.03134700
O	1.47830300	-2.09356000	-1.96304900
O	3.76657300	-2.14213900	-1.07013500
O	1.90620200	-1.33762100	0.32338900
S	-2.29168200	2.30857400	-0.82937700
O	-0.87328500	2.51213900	-1.12974000
O	-2.98332600	1.93814800	-2.23464600
O	-3.01420200	3.50114000	-0.42340000
O	-2.51569600	1.14540100	0.04310100
H	-0.50621300	-3.59096100	-0.13980200
H	-2.52627400	1.17515800	-2.61682300

int3

C	-4.38013400	-0.78767400	0.14639500
C	-4.94676500	0.43844900	0.66965400
H	-5.99635500	0.56069000	0.87521500
C	-3.98564900	1.34033500	0.81225000
C	-1.74475500	0.65179800	1.56197200
H	-1.98937600	-0.14659900	2.26929100
C	-2.67832600	0.75815600	0.36807300
O	-3.02388700	-0.58067600	0.00485500
O	-0.84943200	1.43160700	1.76328000
C	-4.95774500	-1.93760700	-0.16324000
H	-6.01764700	-2.05241500	-0.01013000
H	-4.05956100	2.35401100	1.16587500
H	-4.39240100	-2.76527600	-0.55966800
C	3.02464400	-2.05183200	1.10031700
C	2.69218400	-1.60245100	2.32883100
C	2.64688600	0.09731400	0.95787200
N	2.99411300	-0.97093300	0.25868500
H	3.28615300	-3.03551500	0.76198800
H	2.60328500	-2.11571900	3.26646000
H	2.56873000	1.09598900	0.57278100
N	2.47334500	-0.25627400	2.21813300

C	3.26389100	-0.98217100	-1.17286300
C	2.44805300	-2.00414600	-1.93267600
H	4.32012000	-1.19318100	-1.30970900
H	3.06614100	0.02124600	-1.53632300
C	0.96140100	-1.72900000	-2.05834500
H	2.61340200	-3.00674800	-1.54252200
H	2.84146300	-2.00803400	-2.94627400
H	0.74043800	-0.67903300	-2.22990900
H	0.55196000	-2.31075800	-2.88031900
C	2.10315300	0.63367000	3.30102200
H	1.16045300	0.31318000	3.72835400
H	2.87636000	0.61235100	4.06057100
H	2.00576900	1.63710500	2.90797200
S	-0.01403900	-2.22674700	-0.66805700
O	-1.44844700	-2.28685900	-1.31959300
O	0.36394700	-3.57222800	-0.28969500
O	-0.05035500	-1.21002100	0.36846700
S	1.04232700	2.81833000	-1.05289800
O	0.52655900	1.43979600	-1.16177100
O	0.79389800	3.21128400	0.48325100
O	0.30141400	3.77878900	-1.85889400
O	2.49064300	2.89977000	-1.19445400
O	-2.15231500	1.46017400	-0.67818600
H	-1.20341200	1.26683600	-0.80183300
H	-2.04764600	-1.63182600	-0.88501300
H	0.05007200	2.68667500	0.83709200

TS_{3,4} (imaginary frequency = -657.38 cm⁻¹)

C	-4.62366600	-0.38305700	-0.24678400
C	-4.74265900	1.05306100	-0.12580200
H	-5.62596500	1.56762300	-0.46533700
C	-3.67678300	1.64509900	0.39773900
C	-2.38714500	0.42771000	2.24301500
H	-3.31047700	0.22176900	2.79315300
C	-2.54238200	0.76265500	0.76247800
O	-3.44504200	-0.75920300	0.39172400
O	-1.30023100	0.42967400	2.74975200
C	-5.43422700	-1.25677400	-0.81653400
H	-6.34487200	-0.90734500	-1.27444500
H	-3.56061600	2.70652600	0.54910700
H	-5.20582800	-2.30990400	-0.83928300
C	3.00534600	-2.03330800	1.08990200
C	2.83519700	-1.28243200	2.19879400
C	2.97594900	0.06943600	0.48694400

N	3.09531500	-1.16751800	0.03290000
H	3.07502900	-3.09613500	0.96410600
H	2.72571300	-1.56093000	3.22881700
H	3.02935400	0.96456400	-0.10563000
N	2.83392400	0.02738300	1.80020500
C	3.25809400	-1.53626800	-1.36592000
C	2.20124600	-2.49516700	-1.86539200
H	4.23706600	-1.99278800	-1.47697200
H	3.24903700	-0.61474900	-1.93762400
C	0.78245200	-1.96220700	-1.95531300
H	2.21984500	-3.42102100	-1.29329600
H	2.49803400	-2.76066600	-2.87730500
H	0.73728300	-0.90627400	-2.21125000
H	0.23148600	-2.51686700	-2.71070900
C	2.63851400	1.17323600	2.66666200
H	1.59143100	1.25478200	2.93554600
H	3.23914400	1.04213500	3.55865000
H	2.95629800	2.06646000	2.14395100
S	-0.21841700	-2.16137400	-0.50503000
O	-1.61300300	-2.05569300	-0.96769300
O	0.13960600	-3.39765800	0.16351500
O	0.07852000	-0.97812500	0.41887800
S	1.17419900	2.81774600	-1.11270900
O	1.02790800	1.50737100	-1.74929200
O	0.59412800	2.63974400	0.37962600
O	0.37559600	3.86312100	-1.74556500
O	2.56069000	3.19792400	-0.85113100
O	-1.48875400	0.79611700	0.05571000
H	-0.63317300	-0.10059300	0.28990700
H	-2.84104200	-1.33863800	-0.14827400
H	-0.23990000	2.14294400	0.34605700

int4

C	-4.96873000	-1.10438500	0.30937900
C	-5.13851200	0.04080000	-0.56570100
H	-6.02802000	0.00938600	-1.17871800
C	-4.30880300	1.08078300	-0.73430700
C	-2.99236000	1.02364100	1.50608200
H	-3.92376100	0.91960100	2.06900500
C	-3.10591000	1.37769600	0.02411100
O	-3.75175400	-1.29459100	0.90343900
O	-1.90626200	0.97994500	2.02006900
C	-5.98522300	-1.91993300	0.57962100
H	-6.95992900	-1.73213700	0.15969600

H	-4.51870500	1.79109000	-1.52097300
H	-5.85704600	-2.76301800	1.23981300
C	3.37965500	-2.28635000	0.71165800
C	3.46281800	-1.64024000	1.89438400
C	3.52343400	-0.14223600	0.30484900
N	3.42817200	-1.33102700	-0.26799200
H	3.29680300	-3.33197400	0.48569100
H	3.46354900	-2.01027400	2.90109300
H	3.57755500	0.79845700	-0.20957200
N	3.55909700	-0.30449400	1.61555700
C	3.31062300	-1.56794600	-1.69825400
C	2.04398600	-2.30138800	-2.08197200
H	4.17336000	-2.14805200	-2.01076600
H	3.35697900	-0.59840100	-2.18371000
C	0.74974300	-1.51870900	-1.96323200
H	1.96500000	-3.24853600	-1.55153100
H	2.15206600	-2.55394800	-3.13394800
H	0.87134000	-0.45637100	-2.16103100
H	0.01810500	-1.90755800	-2.66843500
C	3.60081900	0.76556000	2.59215900
H	2.66297400	0.79369800	3.13572400
H	4.41955100	0.59064900	3.28030600
H	3.75120800	1.70341800	2.07409200
S	-0.12350600	-1.64745000	-0.42941200
O	-1.45099200	-1.09781800	-0.67138600
O	-0.01666000	-2.99160700	0.09074200
O	0.61012700	-0.74208000	0.61597500
S	1.25866600	2.65428600	-0.64250300
O	1.52222900	1.65035000	-1.67199400
O	0.35068400	1.87942100	0.46987100
O	0.42751200	3.76484700	-1.08558500
O	2.44440600	3.02989900	0.11702800
O	-2.19655800	2.03626700	-0.45238500
H	0.46339500	0.23650400	0.50195200
H	-3.04195600	-1.33472300	0.24289700
H	-0.60698300	2.02065400	0.28724000

TS₄₋₅ (imaginary frequency = -1385.91cm⁻¹)

C	-2.51105200	0.24798100	-1.45661200
C	-3.72445100	-0.53014300	-1.66655300
H	-3.98698200	-0.71951300	-2.69543500
C	-4.52386900	-0.96683600	-0.69403800
C	-3.02836100	-1.32856500	1.39659600
H	-2.30737400	-1.82964300	0.74403800

C	-4.32301500	-0.81371900	0.76214200
O	-2.29744100	0.60890000	-0.22997700
O	-2.86956600	-1.20160100	2.57967600
C	-1.63871100	0.49861300	-2.50102000
H	-2.06280200	0.41801400	-3.49292200
H	-5.44057900	-1.47544200	-0.96079700
H	-0.89987700	1.27652200	-2.35387900
C	2.92965900	-1.96255400	1.50090500
C	1.98923900	-1.93100300	2.46904600
C	2.20459900	0.09413100	1.67639000
N	3.05381800	-0.68392700	1.02706600
H	3.52381400	-2.77200700	1.12366000
H	1.59717300	-2.70724100	3.09695300
H	2.06629400	1.14528900	1.50028900
N	1.55925600	-0.63514300	2.56778300
C	3.90910600	-0.25476700	-0.06832100
C	3.60168700	-0.96574300	-1.36526700
H	4.93915600	-0.44406400	0.21759700
H	3.77302500	0.81757500	-0.16841300
C	2.25008400	-0.66728300	-1.98979500
H	3.73167800	-2.04010200	-1.24790200
H	4.36024200	-0.64271500	-2.07431800
H	1.92496300	0.35697700	-1.81682900
H	2.30663600	-0.82421400	-3.06315600
C	0.50137600	-0.15565700	3.43286500
H	-0.43992300	-0.60534600	3.13818600
H	0.72945200	-0.41663000	4.45998500
H	0.43794900	0.92080000	3.33731500
S	0.90288800	-1.71638000	-1.48366300
O	-0.08523400	-1.58593100	-2.63712000
O	1.40098700	-3.08560300	-1.41022800
O	0.29364300	-1.19286200	-0.26293400
S	0.57782800	3.03489400	-0.13348900
O	-0.08761300	1.81790000	0.35680100
O	-0.25784600	4.17842700	0.62499900
O	0.41042900	3.27096600	-1.56021300
O	1.95614100	3.13978500	0.33230300
O	-5.18789500	-0.38150700	1.48322600
H	-0.88479300	-0.61516400	-2.49670200
H	-1.44554500	1.11193700	-0.09464500
H	0.07193100	5.04770400	0.36715900
int5			
C	1.94181100	1.96312800	-0.91454800

C	1.49629100	3.32358200	-0.58988300
H	1.36427600	4.01976700	-1.40320300
C	1.27778100	3.69972800	0.66793600
C	0.63410200	1.56253000	2.00542300
H	-0.12376600	1.34699600	1.24368800
C	1.45961400	2.84118000	1.85910300
O	2.17308500	1.17999500	0.00546000
O	0.82041100	0.86908000	2.97031700
C	2.10882700	1.60506300	-2.33727300
H	2.80784000	2.30651600	-2.79170100
H	0.99047200	4.71970700	0.88517400
H	2.47129800	0.59097600	-2.44930800
C	-2.91184200	-0.71315100	1.75203000
C	-1.89834400	-1.00412500	2.59457300
C	-1.63306600	-2.19686000	0.78317600
N	-2.72836000	-1.47241300	0.62792700
H	-3.74462600	-0.04770700	1.86697900
H	-1.66601700	-0.63564800	3.57445100
H	-1.23732500	-2.89210100	0.06800000
N	-1.11676300	-1.93988900	1.97239800
C	-3.62321700	-1.55067900	-0.52095300
C	-4.04971600	-0.21338300	-1.08871500
H	-4.50376400	-2.09626000	-0.19416300
H	-3.11862000	-2.14975500	-1.27217100
C	-3.08894500	0.49404100	-2.02160300
H	-4.35704700	0.46336700	-0.29353100
H	-4.94684500	-0.41702000	-1.66973900
H	-2.68841000	-0.17760100	-2.77781200
H	-3.62175600	1.28948300	-2.53615400
C	0.05627200	-2.56612700	2.54796700
H	0.79074300	-1.80564800	2.78292400
H	-0.22974600	-3.09120600	3.45246200
H	0.46287200	-3.27121800	1.83416600
S	-1.69135600	1.30699500	-1.27464500
O	-1.21025600	2.23978800	-2.31145200
O	-2.20221400	2.00193100	-0.07784300
O	-0.69791600	0.26563500	-0.94542800
S	2.24685600	-2.35566700	-0.98092500
O	2.14279200	-1.34880100	0.19144300
O	2.89570400	-3.57803200	-0.23670700
O	3.14371400	-1.84572100	-1.98519300
O	0.94657600	-2.81831100	-1.37520100
O	2.18794100	3.16869000	2.76476000
H	1.15424600	1.72935800	-2.84448800

H	2.20420900	-0.36876500	-0.05614400
H	3.80374500	-3.39195200	0.04278300
int6			
C	-4.27833900	-0.91358400	0.00358100
C	-4.08612000	-2.29520200	-0.44729600
H	-4.89021600	-2.77381100	-0.98443200
C	-2.94232200	-2.93450500	-0.20557400
C	-1.23811400	-1.02805000	-0.07376400
H	-1.61496600	-0.71315600	-1.04816300
C	-1.79206700	-2.32237000	0.50132700
O	-3.46617000	-0.43710600	0.79794800
O	-0.44772600	-0.37086900	0.56555400
C	-5.42515500	-0.14198000	-0.51655400
H	-6.34676500	-0.63911200	-0.21550500
H	-2.80997900	-3.96201600	-0.51236500
H	-5.40918500	0.87562600	-0.14509300
C	4.37106300	-0.24622300	1.57553800
C	3.69454500	-1.14352400	2.32307800
C	2.34350400	0.51379200	1.87337400
N	3.51294100	0.78741200	1.31771900
H	5.38015100	-0.25036300	1.21171600
H	3.99784500	-2.08083500	2.74720200
H	1.48181500	1.15395900	1.85299900
N	2.43205400	-0.64565900	2.50231800
C	3.80250600	1.93595400	0.47127600
C	3.77422400	1.58892300	-1.00180800
H	4.78210200	2.30524800	0.75557800
H	3.06920900	2.70014900	0.70832700
C	2.38695900	1.23096300	-1.52213400
H	4.48479100	0.78708100	-1.19739800
H	4.14529300	2.45900400	-1.53635000
H	1.61557100	1.34221600	-0.76231100
H	2.10449300	1.85779300	-2.36294000
C	1.37572600	-1.28241800	3.26440300
H	0.47767000	-0.68379000	3.18885900
H	1.18847000	-2.26964100	2.86007700
H	1.67982100	-1.36074800	4.30192500
S	2.26258400	-0.43814600	-2.10736200
O	0.88660100	-0.55287200	-2.64907600
O	3.29498600	-0.59533400	-3.14209700
O	2.47041900	-1.32211300	-0.94603500
S	-2.21537600	2.60519400	0.06171200
O	-3.07527800	2.08018200	1.24820800

O	-0.74056100	2.28717600	0.48109100
O	-2.31998800	4.03411100	0.05934800
O	-2.54515100	1.84910600	-1.12083100
O	-1.28546800	-2.81906400	1.47693600
H	-5.40404300	-0.15208700	-1.60487100
H	-3.31725200	1.11299100	1.11976300
H	-0.53195800	1.32060100	0.40914400
O	-0.16067600	-2.82592200	-1.45043800
H	0.17563800	-2.08977000	-1.98832100
H	0.56485000	-2.99338000	-0.84523800

TS₆₋₇ (imaginary frequency = -690.74 cm⁻¹)

C	4.27622400	-0.79474900	0.44947900
C	4.03293700	-2.04738000	0.98184000
H	4.50813900	-2.34033200	1.90145400
C	3.09806800	-2.87272100	0.38076500
C	1.04325300	-1.26727500	0.38351900
H	1.79297900	-0.77487200	1.01042500
C	2.18836400	-2.46537600	-0.59605900
O	3.68643500	-0.52560600	-0.67949200
O	0.42492000	-0.65223700	-0.52050900
C	5.10791900	0.23543500	1.09975000
H	5.88004200	0.57262600	0.41061100
H	2.79679100	-3.78436600	0.88409800
H	4.49091700	1.09915400	1.34467600
C	-4.44268300	0.00523100	-1.32306900
C	-4.14358000	-1.22493200	-1.79245400
C	-2.30496400	-0.04608700	-1.77931200
N	-3.27971500	0.72755000	-1.33250000
H	-5.37133300	0.42627200	-0.98991100
H	-4.76086200	-2.08726900	-1.95325000
H	-1.28227900	0.25095500	-1.90143200
N	-2.80379200	-1.23227100	-2.07531900
C	-3.09985600	2.07086000	-0.80702500
C	-3.12118300	2.11892600	0.70593700
H	-3.89376700	2.69162600	-1.20815500
H	-2.15268300	2.43619000	-1.19119100
C	-1.94995600	1.41202000	1.38088500
H	-4.07358100	1.74707800	1.08108700
H	-3.07969900	3.16846200	0.98331500
H	-1.12180300	1.21376900	0.70324400
H	-1.56746400	1.99470700	2.21441100
C	-2.04240400	-2.36757300	-2.55568700
H	-0.99017300	-2.11358200	-2.54372000

H	-2.21733600	-3.21311900	-1.90025000
H	-2.35171600	-2.61493200	-3.56511700
S	-2.39287200	-0.14142900	2.09469400
O	-1.08620100	-0.55526200	2.86938100
O	-3.41583200	0.07646000	3.09356900
O	-2.63952000	-1.12880100	1.06196700
S	2.13578200	2.40703600	-0.57286800
O	3.40966300	1.94583900	-1.18743000
O	0.98141400	1.68091300	-1.37592600
O	1.91070600	3.82448300	-0.79553900
O	2.01595300	1.95629300	0.81327800
O	1.81720900	-2.67067900	-1.70610800
H	5.56547100	-0.14853900	2.00336900
H	3.68019700	0.45661100	-0.91558800
H	0.84303800	0.74317600	-1.02291900
O	0.28675800	-2.12227600	1.18126400
H	-0.53756500	-1.16864700	2.31597200
H	-0.44418600	-2.44290900	0.63735000

int7

C	4.40868600	-0.46667200	0.62300500
C	4.34396000	-1.66354400	1.21217700
H	4.83547900	-1.82068300	2.15701600
C	3.62447000	-2.79394000	0.64658900
C	0.89246700	-1.04464500	0.97351500
H	1.73467600	-0.53654000	1.43705100
C	3.01374500	-2.83792100	-0.51568600
O	3.79665100	-0.33195800	-0.57978800
O	0.57339600	-0.94176800	-0.18663800
C	5.10879000	0.72244600	1.16688100
H	5.87644600	1.06901300	0.47549200
H	3.55742600	-3.72513200	1.19207600
H	4.40959500	1.54551200	1.31137300
C	-4.25277200	-0.55891600	-1.45803900
C	-3.89585500	-1.85648800	-1.56702700
C	-2.08822300	-0.64543000	-1.75794000
N	-3.10735400	0.18060000	-1.58934400
H	-5.21158100	-0.10171900	-1.30723300
H	-4.48201300	-2.75400100	-1.52887100
H	-1.06695600	-0.35124000	-1.89701900
N	-2.54064900	-1.88547100	-1.75850500
C	-2.99168600	1.62268600	-1.44441700
C	-3.18440700	2.08948400	-0.01796400
H	-3.73595800	2.08220400	-2.08629200

H	-2.00791600	1.89739000	-1.81007600
C	-2.13034700	1.60035900	0.96899400
H	-4.18558600	1.84158700	0.33068900
H	-3.13300400	3.17456200	-0.03902600
H	-1.20438100	1.28529000	0.48972700
H	-1.88895300	2.37684800	1.68958400
C	-1.72268200	-3.07832300	-1.84484200
H	-0.68972300	-2.78501700	-1.98180400
H	-1.82192300	-3.64447800	-0.92527000
H	-2.04839400	-3.68150000	-2.68458500
S	-2.67252800	0.24191100	1.96377600
O	-1.57995700	0.20782400	3.11305600
O	-3.91873600	0.58999500	2.60444400
O	-2.58507700	-1.00774100	1.23480500
S	1.82960500	2.48543500	-0.81570700
O	3.22065100	2.24444000	-1.24045600
O	0.94646700	1.39074200	-1.58888200
O	1.29904600	3.74972300	-1.29890700
O	1.62159200	2.22050800	0.60649100
O	2.45134800	-2.97059700	-1.52912700
H	5.57514200	0.49227000	2.11919000
H	3.72681600	0.60476000	-0.84045700
H	0.98547400	0.53863200	-1.11024300
O	0.23076900	-1.78248000	1.84511300
H	-0.90532100	-0.46658400	2.92657200
H	-0.50264000	-2.22869100	1.39556200

int8

C	-4.36203300	1.62646100	0.34569500
C	-5.27830500	0.67877800	0.12787400
H	-6.29030600	0.88090800	0.43935600
C	-5.00217900	-0.59736300	-0.51547800
C	-5.80655300	-1.63004100	-0.48638900
O	-3.04150500	1.50640500	0.03952100
C	-4.66827800	2.95699900	0.92547600
H	-5.72626100	3.05455000	1.14447600
H	-4.10195800	-0.77215900	-1.08943500
H	-4.10102200	3.11444800	1.84209700
C	0.20950800	2.92115400	0.10709700
C	0.73044200	3.20212900	-1.10612400
C	2.15533500	1.93243400	-0.04098000
N	1.12174400	2.13620000	0.75959400
H	-0.71900300	3.20864000	0.55973300
H	0.35164500	3.79292100	-1.91733900

H	3.02552600	1.34852900	0.19948600
N	1.94746900	2.58057200	-1.17330200
C	0.92580500	1.51576200	2.05932900
C	-0.04096400	0.35140100	2.01718700
H	0.55011700	2.28200900	2.72929200
H	1.90154600	1.20225700	2.41572600
C	0.47484100	-0.88161500	1.28549500
H	-0.99851600	0.67957000	1.61604100
H	-0.22892700	0.06888800	3.04941700
H	1.55339700	-0.86338600	1.13172900
H	0.23848300	-1.79146900	1.83014300
C	2.86566200	2.63880400	-2.29300000
H	2.35172200	2.32534400	-3.19426200
H	3.23060000	3.65276800	-2.41257600
H	3.69377500	1.97148400	-2.09502300
S	-0.22213700	-1.13164900	-0.31655200
O	0.15686400	-2.45028200	-0.79023300
O	-1.76001400	-1.12155200	-0.03149000
O	0.06717400	0.00628900	-1.16555200
S	4.41096000	-1.14918400	0.17949000
O	4.07439100	-0.43036900	1.40466100
O	5.84127700	-1.79417800	0.56338400
O	4.65239500	-0.27703000	-0.96955400
O	3.53056400	-2.27544800	-0.12200000
O	-6.51349800	-2.55609900	-0.48288300
H	-4.38344600	3.74729200	0.23131700
H	-2.78979000	0.58795200	-0.10948200
H	6.14609000	-2.35277700	-0.16070600
O	-2.93119200	-3.28575500	-0.38118200
H	-2.31592900	-4.02322300	-0.40375000
H	-3.50603900	-3.45698200	0.36884400
H	-2.21867900	-2.04690800	-0.16058500

TS_{8,9} (imaginary frequency = -615.35 cm⁻¹)

C	-5.63346100	0.78062400	-0.20258200
C	-4.82483400	0.33416700	-1.16860400
H	-4.90852000	0.83514800	-2.12126600
C	-3.79516500	-0.70902200	-1.09394800
C	-3.95671100	-1.85612600	-0.34068800
O	-5.65922500	0.29680200	1.07369500
C	-6.60169500	1.89177300	-0.38530800
H	-6.53888400	2.30917100	-1.38492400
H	-3.16980200	-0.83039000	-1.96846500
H	-7.62072500	1.54698800	-0.21203700

C	1.31738400	3.33311600	0.38709800
C	1.85863300	3.49748200	-0.83853500
C	2.89802400	1.84045700	0.13760200
N	1.98925800	2.29954700	0.98254000
H	0.52661800	3.86081900	0.88411100
H	1.63726800	4.19979300	-1.61835200
H	3.57174400	1.02524100	0.32967300
N	2.85144400	2.56396100	-0.96705300
C	1.69052600	1.72942500	2.28567500
C	0.38133200	0.97094700	2.32079100
H	1.65579000	2.54551300	2.99998600
H	2.52157400	1.08391400	2.54845600
C	0.35598700	-0.32521900	1.51994400
H	-0.44142000	1.62485500	2.03752100
H	0.20941000	0.70754300	3.36092600
H	1.35246000	-0.71217600	1.30699900
H	-0.19668300	-1.09796800	2.04689600
C	3.68668500	2.37126300	-2.13564100
H	3.13574600	1.83174200	-2.89818200
H	3.98425300	3.34115200	-2.51527600
H	4.56641000	1.81033400	-1.84953800
S	-0.45322700	-0.21417100	-0.04493000
O	-0.67289800	-1.59324100	-0.53174000
O	-1.82049400	0.39518000	0.31440300
O	0.28060000	0.63487300	-0.95803400
S	3.82595900	-1.78292900	-0.05252300
O	3.90066100	-1.12331800	1.24788800
O	5.00592800	-2.87990500	0.06980100
O	4.18796600	-0.92181600	-1.17758800
O	2.59470200	-2.53755000	-0.27296800
O	-4.74875000	-2.22584400	0.50690800
H	-6.40748400	2.68604800	0.33535600
H	-5.31139800	-0.60704400	1.07974500
H	5.05403700	-3.39127400	-0.74627700
O	-2.85134000	-2.80577100	-0.57014600
H	-1.92621500	-2.34991600	-0.56768100
H	-2.88383500	-3.50851700	0.09714600
H	-2.65638400	-0.07054100	-0.22654700
int9			
C	4.37504400	-0.09289400	-0.13596900
C	4.26200300	1.18369800	-0.49152000
H	4.75925100	1.50799500	-1.39165700
C	3.47094800	2.18207800	0.27940600

C	2.04520800	2.30762400	-0.15798300
O	3.76399200	-0.52087900	1.00301700
C	5.13298100	-1.12301700	-0.88787400
H	5.59999100	-0.69949200	-1.77050900
H	3.41841800	1.90993600	1.33531900
H	5.90483100	-1.56175500	-0.25645000
C	-2.74207500	-3.23762600	0.60586500
C	-3.28391500	-3.15709200	-0.62779300
C	-2.72599400	-1.13688000	-0.00641900
N	-2.40824100	-1.96376600	0.97778400
H	-2.56852400	-4.08035600	1.24643600
H	-3.68513100	-3.91355200	-1.27386800
H	-2.58649200	-0.07000900	0.00219200
N	-3.26935200	-1.83640000	-0.98666000
C	-1.71507800	-1.58425200	2.19791000
C	-0.22644800	-1.85256900	2.12769500
H	-2.15926200	-2.14532200	3.01295800
H	-1.91156500	-0.52987100	2.36194200
C	0.49253400	-1.02266700	1.06753400
H	-0.05289700	-2.91855700	1.98799800
H	0.18826200	-1.60315900	3.09978500
H	-0.13685700	-0.25354000	0.62519600
H	1.37765200	-0.53487200	1.46444300
C	-3.76149100	-1.29465000	-2.23786600
H	-3.21057400	-1.73439900	-3.06119800
H	-4.81675500	-1.52003300	-2.34005400
H	-3.61553900	-0.22251000	-2.23287700
S	1.07903300	-2.02740000	-0.26028800
O	1.71444600	-1.01210700	-1.26078700
O	2.13059200	-2.90262500	0.23497800
O	-0.03475400	-2.67935500	-0.92404400
S	-2.06718200	2.86662400	0.03912500
O	-1.54981700	1.97972400	1.06940100
O	-2.88528700	3.95120600	0.89980900
O	-3.02350600	2.25942800	-0.87790100
O	-1.02047500	3.62856700	-0.66529000
O	1.39465500	1.41692200	-0.69122700
H	4.46680500	-1.92840000	-1.19667000
H	3.75034200	-1.48120500	1.02833900
H	-3.30540200	4.58621900	0.30734600
O	1.51284800	3.46829300	0.10633500
H	1.69706400	-0.03495600	-0.97297700
H	0.56031000	3.48499500	-0.16648500
H	3.91576800	3.17250100	0.23929000

TS_{9-P} (imaginary frequency = -1117.65 cm⁻¹)

C	4.25237700	-0.45186500	-1.25989000
C	4.11628200	0.89434600	-1.57912200
H	4.04623900	1.11894600	-2.63458600
C	4.71434200	1.96577700	-0.71289500
C	4.30793600	1.93320200	0.72721600
O	4.53963000	-0.76843700	-0.03311400
C	3.90202700	-1.52331300	-2.20972500
H	3.40998200	-1.13594000	-3.09341100
H	5.79904600	1.94531900	-0.77656600
H	4.84109100	-1.99262500	-2.50626800
C	-2.07462800	-3.24441600	1.09201000
C	-2.56225400	-3.51784700	-0.13658900
C	-2.69992000	-1.35816000	0.17682000
N	-2.18232500	-1.89223700	1.27194300
H	-1.67068600	-3.88825400	1.84906800
H	-2.67484200	-4.44641700	-0.66159300
H	-2.89841200	-0.31130900	0.02623500
N	-2.95562900	-2.32692900	-0.68480300
C	-1.68864500	-1.15013000	2.42095200
C	-0.18561600	-0.96634300	2.40358200
H	-1.98944900	-1.69576800	3.30914900
H	-2.19695700	-0.19159000	2.42323000
C	0.32324600	-0.06237900	1.28708400
H	0.30596100	-1.93778900	2.37672600
H	0.08198100	-0.51774100	3.35648900
H	-0.47595000	0.50689200	0.81502700
H	1.06361400	0.64523000	1.64860000
C	-3.52457000	-2.15332900	-2.00580200
H	-2.80719200	-2.47694000	-2.75141800
H	-4.43119600	-2.74174700	-2.08766800
H	-3.75419600	-1.10547900	-2.14914700
S	1.14813900	-0.92696300	-0.01531200
O	1.59841400	0.14635700	-0.96146900
O	2.29579900	-1.62866700	0.61672300
O	0.21580100	-1.85082300	-0.65344900
S	-3.76198800	2.37210400	-0.38938700
O	-2.76525100	1.94315600	0.58749700
O	-4.83952800	3.12208200	0.55349400
O	-4.48708000	1.26998800	-1.02121900
O	-3.28509000	3.37251100	-1.33919300
O	3.22369700	1.60140000	1.14133600
H	3.29658400	-2.28868300	-1.73133100
H	3.79569500	-1.37003800	0.30647000

H	-5.57851700	3.42787200	0.01504400
O	5.26944100	2.38489600	1.52222200
H	2.88135600	0.59074600	-1.23393700
H	4.93255600	2.40403800	2.42612500
H	4.40041900	2.94022200	-1.08550300
P			
C	-5.04221500	0.37214700	-1.29875200
C	-4.66320500	-1.07636300	-1.39147800
H	-5.02476000	-1.46218100	-2.34374600
C	-5.20128300	-1.90262100	-0.25416400
C	-4.60738400	-1.56683400	1.06980800
O	-5.66842600	0.79653700	-0.34743000
C	-4.60594500	1.25217100	-2.41990100
H	-3.54162700	1.11861500	-2.60378800
H	-6.28091300	-1.80890700	-0.16521500
H	-5.12595500	0.95789000	-3.33063100
C	2.01678000	3.15638700	1.33532700
C	2.61713200	3.57482200	0.20119100
C	2.84962500	1.40352100	0.32324200
N	2.18293100	1.79954800	1.39715300
H	1.49706600	3.70014700	2.10017700
H	2.73050400	4.55639500	-0.21634400
H	3.13483700	0.39044000	0.09814500
N	3.13164300	2.46496900	-0.41246900
C	1.62888300	0.92603500	2.41927800
C	0.15772600	0.63523500	2.21219600
H	1.78085300	1.41404100	3.37598300
H	2.21014200	0.01007000	2.40954600
C	-0.13551700	-0.19989900	0.97258500
H	-0.40410200	1.56780300	2.20699500
H	-0.17883500	0.08126200	3.08386800
H	0.75881800	-0.64285800	0.53653900
H	-0.82169600	-1.01631500	1.18471400
C	3.89115100	2.45919200	-1.64734300
H	3.28803900	2.87905800	-2.44399100
H	4.79073500	3.05009000	-1.51769300
H	4.15534400	1.43758300	-1.88629300
S	-0.90045500	0.70069900	-0.33892000
O	-1.12696800	-0.20985400	-1.44466600
O	-2.27924300	1.14207700	0.27459400
O	-0.19349100	1.93472600	-0.60117500
S	4.13004300	-2.25163800	-0.47265000
O	3.16635500	-2.01122200	0.60318400

O	5.42641600	-2.90457500	0.23825400
O	4.68956500	-1.03443900	-1.04839200
O	3.66834600	-3.23208900	-1.45063200
O	-3.64173100	-0.85196300	1.26716800
H	-4.82199700	2.29099700	-2.19646000
H	-2.84728900	0.36623800	0.53238900
H	5.17714000	-3.73923400	0.65088500
O	-5.22022700	-2.17302300	2.06601100
H	-3.57577000	-1.13407000	-1.44461800
H	-4.77846500	-1.94566200	2.89368100
H	-4.99677500	-2.96014100	-0.41908700

int4'

C	4.78886600	0.00355600	-0.55303200
C	5.34422100	1.31869500	-0.30578100
H	6.32482900	1.61486200	-0.63680000
C	4.47492700	2.03928500	0.38920500
C	2.05083100	1.80093900	-0.03499000
H	2.01795900	1.69318900	-1.12249500
C	3.25824800	1.21282800	0.67101900
O	3.53501000	-0.02518700	0.01608800
O	1.19971900	2.38850500	0.58938000
C	5.30030900	-1.03305000	-1.19837400
H	6.27738800	-0.94664400	-1.64331200
H	4.57013100	3.04952700	0.74731600
H	4.75812500	-1.95903000	-1.29626600
C	-4.44870600	-0.43247800	0.37235100
C	-4.10667300	-0.82107300	1.61896800
C	-2.61331100	-1.61763900	0.23545000
N	-3.50413700	-0.94724400	-0.47632200
H	-5.27869100	0.14863200	0.01978600
H	-4.57531400	-0.63966600	2.56668600
H	-1.75231900	-2.13353100	-0.15323800
N	-2.96626400	-1.56921800	1.50696700
C	-3.43407100	-0.74074800	-1.91467500
C	-3.37985100	0.71988300	-2.29599100
H	-4.30675200	-1.20314500	-2.36496600
H	-2.55035200	-1.26566200	-2.26335100
C	-2.11994100	1.46818300	-1.89818700
H	-4.26226400	1.24499900	-1.93466300
H	-3.42900200	0.75564900	-3.38154800
H	-1.22060600	0.86307800	-1.98817800
H	-2.00609400	2.34696500	-2.52705900
C	-2.21192600	-2.13808200	2.60521600

H	-1.84787100	-1.34258000	3.24417300
H	-2.85148400	-2.80285900	3.17465000
H	-1.37682200	-2.69494800	2.19870900
S	-2.11699600	2.13630600	-0.25470300
O	-1.04673600	3.27865900	-0.37428700
O	-3.39039600	2.77536500	-0.00487900
O	-1.63590400	1.16834300	0.71618900
S	0.99592300	-2.31579900	-0.71361200
O	0.39571500	-1.00788800	-0.98676100
O	1.83386400	-2.12518200	0.65321200
O	1.95778500	-2.74006300	-1.72555200
O	0.02651200	-3.34090400	-0.33569400
O	3.04835800	1.06038000	2.01219400
H	2.14143200	0.71281000	2.16288500
H	-0.15134200	2.96399100	-0.06385800
H	2.53159000	-1.46051800	0.50019300
O	0.58552000	-0.02803400	2.34562700
H	0.74850000	-0.84135000	1.85701200
H	-0.02416400	0.46960300	1.79164800

TS_{4'-5'} (imaginary frequency = -339.25 cm⁻¹)

C	4.61479900	-0.13974200	-0.28332900
C	5.03184200	1.22415600	-0.53097900
H	5.90103200	1.47862100	-1.11272400
C	4.19337400	2.05400300	0.07384400
C	1.79923300	1.53370900	0.17600000
H	1.44576400	0.87364400	-0.61168800
C	3.14790300	1.25936200	0.79446000
O	3.48571200	-0.08913600	0.50921700
O	1.27826100	2.64553200	0.36124000
C	5.13071100	-1.28541100	-0.69953000
H	6.00328800	-1.27313100	-1.33084300
H	4.20203400	3.12956200	0.09720300
H	4.69167100	-2.23185400	-0.42819000
C	-4.32751100	-0.49223900	1.11056900
C	-3.61797200	-0.84794400	2.20227500
C	-2.56651800	-1.60481500	0.44102500
N	-3.65822200	-0.98550400	0.02280700
H	-5.24462500	0.05578100	1.01453000
H	-3.79417500	-0.67362700	3.24597300
H	-1.84221300	-2.09562900	-0.18480400
N	-2.52945700	-1.54992300	1.76079500
C	-4.03195300	-0.78816000	-1.36826300
C	-3.86048600	0.64084700	-1.83271100

H	-5.06909500	-1.08987100	-1.47351000
H	-3.42200600	-1.46394400	-1.95873400
C	-2.42356500	1.14033300	-1.87534000
H	-4.48127600	1.31010700	-1.23948500
H	-4.25629400	0.68062500	-2.84422300
H	-1.69323600	0.33469200	-1.92928100
H	-2.27472800	1.78408700	-2.73784900
C	-1.49177400	-2.11687300	2.59848300
H	-0.98585700	-1.32474600	3.13772800
H	-1.93668200	-2.81190300	3.30158900
H	-0.78579100	-2.64217800	1.96787000
S	-1.95137900	2.16067100	-0.50406800
O	-0.67411600	2.81163100	-0.99833600
O	-3.00044900	3.15138900	-0.29870300
O	-1.66672700	1.32261500	0.66796400
S	0.92712500	-2.30240100	-0.99055900
O	0.23980400	-1.01808500	-1.15864100
O	1.67743600	-2.19600000	0.43879500
O	1.97529300	-2.53607500	-1.97655700
O	0.01977600	-3.42342100	-0.77466100
O	3.14948600	1.52268600	2.14275200
H	2.33596500	1.14336000	2.50070400
H	0.33136100	2.75815300	-0.25815900
H	2.38786700	-1.52828600	0.39685300
O	0.75892000	0.32257900	1.62254500
H	0.78459000	-0.60481900	1.36050900
H	-0.13144400	0.63397000	1.39140000
int5'			
C	-4.47159700	-0.62696000	-0.34787900
C	-4.71710800	-2.01947300	-0.02636900
H	-5.62019100	-2.53634500	-0.30204400
C	-3.67623100	-2.50235500	0.63747300
C	-1.31608500	-1.71161400	0.13411400
H	-1.44463000	-1.70246100	-0.94652300
C	-2.65404500	-1.43204800	0.81547900
O	-3.23109600	-0.30504500	0.14831400
O	-0.84794800	-2.92252000	0.59880000
C	-5.22288600	0.24897100	-0.99846800
H	-6.18175300	-0.05761400	-1.38139400
H	-3.53390800	-3.49600300	1.02398700
H	-4.89309800	1.26250400	-1.16006900
C	3.95307900	0.93795700	1.50509500
C	3.03845000	0.96595500	2.49736200

C	2.05985800	1.64170900	0.66219800
N	3.32215800	1.37207000	0.37014600
H	4.98673200	0.65109900	1.50655000
H	3.11752600	0.71711000	3.53780700
H	1.32193100	2.01080400	-0.02705200
N	1.86678200	1.41318100	1.95011100
C	3.90027700	1.40604800	-0.96382300
C	4.05540300	0.02835700	-1.57104300
H	4.87014100	1.88574400	-0.88633400
H	3.25866200	2.03307100	-1.57413800
C	2.74249800	-0.67730400	-1.88962200
H	4.68638800	-0.58899300	-0.93422100
H	4.60211000	0.15814600	-2.50059800
H	1.87097500	-0.02552900	-1.83157100
H	2.75867800	-1.10413700	-2.88953400
C	0.62008100	1.59535100	2.66551600
H	0.35805100	0.67159100	3.16833300
H	0.73377600	2.39081000	3.39368600
H	-0.15521700	1.85768500	1.95740900
S	2.38206400	-2.06398500	-0.85607700
O	1.17206200	-2.69263000	-1.36886900
O	3.56271000	-2.88174700	-0.69510100
O	2.06348500	-1.46059400	0.55222200
S	-1.42438200	2.57982600	-0.89112800
O	-0.73135000	1.31391100	-1.21183200
O	-2.31448400	2.25190600	0.39724600
O	-2.33386600	2.99674900	-1.95042100
O	-0.52581700	3.62251500	-0.41429800
O	-2.45353200	-1.15122800	2.15400400
H	-1.62823300	-0.65419200	2.21276700
H	-0.15406900	-3.20890600	-0.00730900
H	-2.70525100	1.35807300	0.31675700
O	-0.40514500	-0.70035900	0.51454400
H	-0.50929100	0.08053800	-0.07299600
H	1.10487400	-1.14842000	0.59289100
int6'			
C	-3.64809600	0.57419600	0.12505200
C	-3.50739500	0.39932600	-1.31051100
H	-3.75596300	1.16354600	-2.02654300
C	-3.03205900	-0.81680900	-1.53928700
C	-1.44481800	-1.97335400	0.07843400
H	-0.82958100	-1.08984500	0.23125800
C	-2.86978600	-1.53827200	-0.24215000

O	-3.26525900	-0.58108400	0.73626300
O	-0.99420600	-2.73167500	-0.99816600
C	-4.06706000	1.63903700	0.80797800
H	-4.39154500	2.51644600	0.27221900
O	-3.64671100	-2.68382600	-0.13489900
H	-4.14925000	1.61822000	1.88296400
C	2.74462600	-1.45787100	2.14466500
C	1.48426400	-1.52667600	2.62382100
C	1.81567500	0.50641700	1.89260800
N	2.93522000	-0.17609400	1.70307500
H	3.51406400	-2.20224600	2.07627600
H	0.93762700	-2.33971900	3.05999900
H	1.66568400	1.54226200	1.64440900
N	0.92612400	-0.28687200	2.46256600
C	4.11775800	0.32883800	1.02198100
C	4.18021800	-0.08639000	-0.43348300
H	4.98510600	-0.04620800	1.55413900
H	4.10184200	1.40991600	1.11479200
C	3.04221700	0.48758500	-1.27320500
H	4.21555100	-1.17262400	-0.49455300
H	5.12458400	0.27506300	-0.82863100
H	2.42624400	1.19602800	-0.72060200
H	3.39796400	0.99442400	-2.16536300
C	-0.40175900	0.10940900	2.89208200
H	-1.08585600	-0.70730400	2.70402200
H	-0.38849000	0.34054200	3.95208700
H	-0.70821000	0.98156800	2.32847700
S	1.94550000	-0.77205500	-1.84710200
O	0.69281500	0.01482800	-2.34991700
O	2.49868900	-1.44108200	-3.00348700
O	1.57663600	-1.60400200	-0.70980100
S	-0.28614200	2.74613100	-0.27194200
O	0.95852200	3.32485100	0.20903100
O	-0.24617700	1.26229300	-0.33397700
O	-0.82402000	3.33533300	-1.48669800
O	-1.30895900	3.05378900	0.91530000
H	-4.53338200	-2.49188000	-0.44953300
H	-0.03202000	-2.68793000	-0.97921800
O	-1.41373500	-2.69042600	1.27352200
H	-2.08745600	-3.37511800	1.21093600
H	-2.13273800	2.54388800	0.79078200
H	0.25124400	0.52097700	-1.59348300
H	-2.80803300	-1.27908400	-2.48448800

TS_{6'-7} (imaginary frequency = -1414.43 cm⁻¹)

C	-3.57973700	0.30342900	-0.02747800
C	-3.33607600	0.02942500	-1.42868800
H	-3.54678300	0.72950200	-2.21723600
C	-2.81999600	-1.19038000	-1.51202000
C	-1.27788900	-2.05977300	0.30735000
H	-0.73724400	-1.12163900	0.40587100
C	-2.71143500	-1.78230500	-0.14790600
O	-3.24518800	-0.74086000	0.70273900
O	-0.69822900	-2.88159500	-0.64918400
C	-4.00792400	1.47718700	0.54512500
H	-4.52385800	2.15786700	-0.11800100
O	-3.41938800	-2.94264600	0.04462000
H	-4.34608300	1.43310900	1.57156800
C	3.01301600	-1.35760600	1.96697700
C	1.81045800	-1.35665300	2.58212300
C	2.15418700	0.64156000	1.76687600
N	3.21403800	-0.09645800	1.47581000
H	3.73652700	-2.13908500	1.83837500
H	1.28932500	-2.13150400	3.10908000
H	2.02500100	1.67959500	1.52010100
N	1.29707800	-0.09410000	2.45266300
C	4.34314400	0.34111800	0.66778200
C	4.20711600	-0.02685900	-0.79589400
H	5.23324400	-0.11096500	1.09166900
H	4.41961700	1.41720000	0.78948200
C	3.00932700	0.62820200	-1.47359700
H	4.16647100	-1.11016400	-0.89383800
H	5.12193600	0.29746400	-1.28375500
H	2.51563300	1.35665700	-0.83311200
H	3.28820600	1.14617000	-2.38673200
C	0.04459200	0.38041700	3.00845200
H	-0.77055500	-0.23546900	2.64912100
H	0.09030000	0.33208000	4.09077200
H	-0.10626700	1.40578700	2.69576000
S	1.76290300	-0.54134200	-1.94790400
O	0.53794400	0.26712100	-2.21885000
O	2.23443800	-1.23987100	-3.14270000
O	1.57413000	-1.43013200	-0.78278700
S	-0.74158500	2.75509200	-0.09262100
O	0.47948900	3.31405800	0.45664700
O	-0.61119900	1.19166200	-0.14823700
O	-1.11745100	3.22136300	-1.41352100
O	-1.86279000	2.90404400	0.91262200

H	-4.29151500	-2.86605600	-0.35214400
H	0.20728300	-2.55331500	-0.77510500
O	-1.29702900	-2.64239700	1.57120800
H	-1.87978500	-3.40636600	1.52634100
H	-2.82880700	2.16828100	0.69137200
H	-0.15846300	0.86094900	-0.99390800
H	-2.51359300	-1.72871800	-2.39166100
,			
int7'			
C	4.03130600	0.20103700	0.54365300
C	3.27579800	0.17776800	1.76006600
H	3.29995300	0.95606300	2.50126700
C	2.57288800	-0.95649900	1.74759900
C	1.62786600	-1.74128000	-0.47169700
H	1.32391200	-0.72440000	-0.71071500
C	2.83960800	-1.70011200	0.48996400
O	3.84342800	-0.84751500	-0.16397100
O	0.62426100	-2.46195100	0.14731900
C	4.92091000	1.24317600	0.05841800
H	5.49853100	1.64398800	0.88704100
O	3.31611600	-2.96443900	0.59518500
H	5.55554600	0.87998900	-0.74015900
C	-3.75168100	-1.98737500	-0.27580200
C	-2.79974200	-2.58764400	-1.02164700
C	-2.80343700	-0.46006900	-1.51878700
N	-3.74706900	-0.66141600	-0.61301600
H	-4.42672000	-2.38502800	0.45715700
H	-2.48873400	-3.61282500	-1.07683700
H	-2.55107500	0.48263300	-1.96562100
N	-2.22718900	-1.61604500	-1.79592700
C	-4.52390500	0.38223300	0.03739000
C	-3.95275300	0.79155900	1.37882400
H	-5.53329000	0.00363500	0.15871400
H	-4.55891500	1.22662800	-0.64368000
C	-2.58446000	1.45922100	1.30324000
H	-3.92698000	-0.06977300	2.04441000
H	-4.66230700	1.49017200	1.81425100
H	-2.29533200	1.71165600	0.28450500
H	-2.55977300	2.37768400	1.88281200
C	-1.17788600	-1.82554800	-2.77285500
H	-0.45172800	-2.51451400	-2.36125400
H	-1.60017200	-2.23494300	-3.68449000
H	-0.70121800	-0.87689400	-2.98300300
S	-1.28052900	0.45682400	1.96288900

O	-0.05556600	1.28845800	1.87489800
O	-1.63735300	0.14485700	3.35067300
O	-1.21250600	-0.74364400	1.10502700
S	0.53220600	2.56251400	-1.37151700
O	-0.28685100	1.44885100	-1.86572000
O	1.44025100	1.95301900	-0.20133500
O	-0.26962800	3.62066400	-0.75466400
O	1.52092800	3.03932700	-2.33264900
H	3.97164700	-3.02639200	1.29615600
H	-0.01430900	-1.83658800	0.53808000
O	2.02666800	-2.35148900	-1.64703400
H	2.34798700	-3.23192400	-1.42717800
H	4.29382500	2.05503000	-0.31667900
H	0.86062000	1.65626000	0.54272000
H	1.88644400	-1.32552900	2.49112300

TS_{7,-8'} (imaginary frequency = -527.72 cm⁻¹)

C	-3.80648700	-0.52225900	-0.26218700
C	-2.89673600	-0.01889500	-1.16972200
H	-2.76539500	1.02008000	-1.40450300
C	-2.17773000	-1.09968200	-1.64590600
C	-1.28426900	-2.14894600	0.56280500
H	-1.62330500	-1.18004500	0.92769500
C	-2.59826600	-2.22133100	-0.93180900
O	-3.70209300	-1.84046100	-0.17668400
O	-0.08246200	-2.27807100	0.08427900
C	-4.77330400	0.14879800	0.61551100
H	-4.81047500	1.20667500	0.38387600
O	-2.53832400	-3.52187900	-1.24582600
H	-5.76230300	-0.28616800	0.49031000
C	3.66460700	-1.62768400	-0.20231900
C	2.98773300	-2.51584800	0.55615200
C	3.07720600	-0.62743900	1.64919400
N	3.71604000	-0.45677700	0.50501700
H	4.12568900	-1.73609500	-1.16457000
H	2.73320000	-3.54297600	0.38154300
H	2.94276000	0.12131400	2.40658200
N	2.63785800	-1.87175200	1.71212600
C	4.34888300	0.78141500	0.07438400
C	3.86615900	1.27663700	-1.26914300
H	5.41877600	0.60130600	0.02831700
H	4.16466200	1.51611000	0.85130300
C	2.46558200	1.85326800	-1.33312800
H	3.98811000	0.50336400	-2.02557200

H	4.54581900	2.07886900	-1.54766600
H	2.21289200	2.45125200	-0.45983400
H	2.38742800	2.49610200	-2.20617200
C	1.89058700	-2.45096600	2.80998200
H	0.89571900	-2.71865300	2.47407900
H	2.40832900	-3.33408600	3.16676500
H	1.82324900	-1.72230100	3.60778700
S	1.13112600	0.70031500	-1.56057600
O	0.00383100	1.53000100	-2.04474100
O	1.55912300	-0.30073800	-2.54092900
O	0.81350900	0.10091200	-0.23592200
S	-1.19327000	3.03481900	1.09218400
O	-1.70091000	1.72093500	1.49820800
O	-1.42882400	3.14189900	-0.48831000
O	0.25063400	3.17689100	1.29752800
O	-1.97824300	4.15360000	1.60525800
H	-2.94663600	-3.67060800	-2.10386400
H	0.30917600	-1.38208000	-0.14242300
O	-1.71878300	-3.16967000	1.27190100
H	-1.21191300	-3.96105600	1.05206700
H	-4.48239900	0.02401100	1.65671800
H	-0.88101800	2.47982000	-0.97496700
H	-1.35880600	-1.09704000	-2.34419300

int8'

C	-3.86823700	-0.66788300	-0.84031700
C	-2.81623900	-0.93296700	-1.64020000
H	-2.35854300	-0.24149100	-2.32410200
C	-2.44254900	-2.29955900	-1.42860400
C	-1.32027700	-0.71740100	1.62223300
H	-1.49421000	0.35560800	1.63508200
C	-3.30413900	-2.75273300	-0.49753200
O	-4.17643000	-1.80268600	-0.12478800
O	-0.35542900	-1.24006500	1.09238400
C	-4.72068700	0.51078700	-0.60187000
H	-4.42557400	1.31176000	-1.27187900
O	-3.39901100	-3.93653300	0.11129500
H	-5.77019100	0.28360900	-0.78273800
C	3.35215200	-2.09254000	0.16835500
C	2.71822600	-2.24208400	1.35078400
C	3.72189900	-0.30139900	1.36728700
N	3.97798900	-0.87437200	0.20348400
H	3.42013900	-2.74406400	-0.68107800
H	2.12112200	-3.04595100	1.73497100

H	4.06700200	0.66729700	1.67535800
N	2.97325700	-1.11677500	2.08771600
C	4.72360400	-0.26657100	-0.88796800
C	3.91119000	-0.11802100	-2.15485000
H	5.58925400	-0.89053300	-1.08705700
H	5.07423500	0.69688500	-0.53355400
C	2.76508700	0.87643400	-2.11681400
H	3.55505800	-1.08703100	-2.49981400
H	4.60233500	0.23731900	-2.91518000
H	2.95610700	1.74003300	-1.48337900
H	2.56331700	1.24281600	-3.12068400
C	2.43480000	-0.82524800	3.40080400
H	1.37034200	-0.63141900	3.32289800
H	2.60930400	-1.67278100	4.05282600
H	2.93842500	0.04728200	3.79680200
S	1.18885800	0.23956400	-1.62517400
O	0.17825500	1.18664400	-2.08859300
O	1.02690200	-1.13782600	-2.05115300
O	1.25835800	0.31307600	-0.07162800
S	-1.01837700	3.29726600	0.67989500
O	-0.52418700	2.53097400	1.82616800
O	-1.70709300	2.22516700	-0.30631900
O	0.05012000	3.91352000	-0.10661400
O	-2.12522000	4.18848200	1.00991500
H	-4.22547700	-3.98236500	0.59964800
H	0.60227700	-0.32122600	0.38878400
O	-2.24406700	-1.38777000	2.24719200
H	-2.05898200	-2.33623500	2.19592900
H	-4.63083800	0.87320700	0.42139800
H	-1.03409700	1.84766000	-0.90090800
H	-1.64399900	-2.85040500	-1.88798300

int9'

C	2.67279300	-1.95025200	1.38288300
C	1.46434200	-2.36807900	0.96523300
H	0.63392500	-2.63412800	1.59366800
C	1.47930700	-2.36232900	-0.47337100
C	2.72757200	-1.95280500	-0.80479100
O	3.46282600	-1.69835800	0.28119300
C	3.29381800	-1.71570200	2.69736200
H	2.57479100	-1.93716500	3.47960500
O	3.30257100	-1.79700400	-1.98876700
H	4.16535500	-2.35188800	2.84337700
C	0.99790000	2.13996300	1.84794400

C	0.57706500	1.11515700	2.61966400
C	-1.18471400	2.05802600	1.73467500
N	-0.12010500	2.72268700	1.31386200
H	1.98373600	2.50435000	1.63541100
H	1.12033200	0.42144300	3.23134200
H	-2.20335800	2.28702100	1.48576700
N	-0.78995200	1.09067600	2.54292100
C	-0.13107000	3.79279400	0.32894000
C	0.28966800	3.31357800	-1.04431200
H	0.54841100	4.56353300	0.67637500
H	-1.13467400	4.20473100	0.31254500
C	-0.70349700	2.35481200	-1.69388600
H	1.28086000	2.86767400	-0.98155600
H	0.38942200	4.19095400	-1.67574600
H	-1.60067600	2.17739700	-1.10200500
H	-1.02457300	2.69848300	-2.67403900
C	-1.65747700	0.15149300	3.22525800
H	-1.54982900	-0.83097900	2.78227800
H	-1.38353600	0.11839800	4.27314800
H	-2.68109900	0.48879600	3.12985300
S	-0.02774300	0.76152700	-1.99922200
O	-1.02020600	-0.07475200	-2.65408800
O	1.26047900	0.85310100	-2.66237900
O	0.18640500	0.29038200	-0.51610200
S	-3.16001800	-1.47681100	-0.09034100
O	-1.96221200	-2.15225300	0.41379400
O	-3.11632200	-1.63718200	-1.68925000
O	-3.15370700	-0.03311300	0.16030400
O	-4.40973600	-2.14036800	0.25992400
H	4.13481500	-1.32298400	-1.89566200
H	0.74630800	-0.52198400	-0.46494600
H	3.61564500	-0.68121100	2.80611000
H	-2.36574100	-1.12205400	-2.03177600
H	0.71239900	-2.68867800	-1.15188200
O	3.37783600	1.28428500	-0.66500700
H	4.13416700	0.70047500	-0.61834700
H	2.90018200	1.00096800	-1.44854800

TS_{9-10'} (imaginary frequency = -1427.14 cm⁻¹)

C	3.49744000	-1.27063300	1.35203800
C	2.27949800	-1.20628200	1.88891800
H	2.02651200	-0.72145000	2.81333100
C	1.34475600	-1.84403600	0.96774900
C	2.18457900	-2.36348200	-0.01634000

O	3.42357200	-1.98149400	0.14305900
C	4.83626800	-0.78352100	1.71110600
H	4.78448900	-0.27136100	2.66591500
O	1.86458700	-3.07979000	-1.04488600
H	5.54256100	-1.60724900	1.79322700
C	0.84269800	2.81914400	1.10263600
C	0.47339400	2.10732700	2.18831500
C	-1.30616900	2.43707400	0.96443900
N	-0.28774200	3.02525200	0.35804800
H	1.80037300	3.19169000	0.79613900
H	1.04001600	1.75605400	3.02835300
H	-2.32019000	2.42536000	0.61369900
N	-0.87323800	1.88427400	2.08293400
C	-0.33889200	3.65251600	-0.95207100
C	0.19011500	2.75396700	-2.04973800
H	0.25088800	4.56164400	-0.90017200
H	-1.37214600	3.92911800	-1.13488600
C	-0.66671900	1.52284900	-2.32243700
H	1.21903100	2.47502700	-1.82943200
H	0.22690600	3.35394000	-2.95464500
H	-1.63097900	1.54645200	-1.81811600
H	-0.85905400	1.40058800	-3.38534700
C	-1.68769200	1.16935800	3.04556600
H	-1.27411800	0.17980500	3.19777900
H	-1.70047300	1.71353300	3.98315300
H	-2.69341100	1.08699500	2.65574900
S	0.08812300	-0.00145500	-1.84628400
O	-0.78997700	-1.09075200	-2.28573500
O	1.43529600	-0.06674800	-2.41742700
O	0.15771200	0.08069500	-0.33338100
S	-3.29889900	-1.39606300	0.34346000
O	-2.24785700	-1.76937300	1.29292800
O	-2.96355700	-2.16678500	-1.02270400
O	-3.28239500	0.02967200	0.00274100
O	-4.61785100	-1.91430000	0.68923400
H	2.61577900	-3.21253900	-1.63702700
H	0.78062600	-0.83925900	0.23814400
H	5.21147200	-0.08864800	0.96317600
H	-2.16991200	-1.76572300	-1.42940800
H	0.43286100	-2.34650000	1.25266100
O	3.38421600	1.32226800	-0.82752100
H	4.00864600	1.60201400	-1.49722100
H	2.77378800	0.75129400	-1.30831300

int10'

C	2.82949800	-2.07161900	0.94177800
C	2.22555900	-1.62365800	2.02830000
H	2.70239500	-1.09890300	2.83518700
C	0.79175600	-2.00897100	1.98805500
C	0.73320200	-2.65844700	0.67532800
O	1.87467300	-2.72674300	0.10186100
C	4.19988300	-2.11316700	0.42325200
H	4.84865400	-1.54787300	1.08255500
O	-0.29959300	-3.15411100	0.14621200
H	4.55113400	-3.14222700	0.37728400
C	1.13690600	2.65942400	1.35235700
C	0.50153900	2.04908100	2.37519800
C	-1.00669100	2.67502400	0.92372500
N	0.17417500	3.05241600	0.46312100
H	2.18006000	2.83038400	1.17243000
H	0.87946400	1.60575900	3.27583600
H	-1.94957700	2.86201600	0.44722700
N	-0.83780500	2.07994300	2.09109500
C	0.40425200	3.69575500	-0.82077000
C	0.98402600	2.75199000	-1.85058100
H	1.08165000	4.52654000	-0.65180500
H	-0.54911400	4.09746800	-1.14812100
C	0.06574100	1.59801400	-2.23626000
H	1.94640900	2.38425500	-1.50050100
H	1.19176900	3.34808200	-2.73519800
H	-0.94723700	1.72397500	-1.85812900
H	0.00386600	1.49156500	-3.31551100
C	-1.89885300	1.57617100	2.93987100
H	-1.65568500	0.56969500	3.25708900
H	-2.00617000	2.21748100	3.80762200
H	-2.82080800	1.56787200	2.37329400
S	0.63127500	0.01773300	-1.65376200
O	-0.22558100	-0.99601700	-2.31606900
O	2.03760200	-0.09925000	-2.09156000
O	0.48542200	-0.00679500	-0.19196500
S	-3.21336900	-0.87040000	-0.24436800
O	-2.52918000	-1.21186000	1.00524500
O	-2.57916200	-1.79464500	-1.38389700
O	-2.96423200	0.51073100	-0.66937300
O	-4.62216000	-1.25583700	-0.26101100
H	-0.14369000	-3.50619200	-0.74417700
H	0.07305100	-1.19271900	2.03061800
H	4.25269800	-1.69256200	-0.57647400

H	-1.68293400	-1.46258800	-1.63275500
H	0.51191800	-2.73264900	2.75683900
O	3.82654000	1.15741500	-0.27308600
H	4.42419800	1.61872300	-0.86155800
H	3.23133600	0.68737700	-0.87354100

TS_{10'-11'} (imaginary frequency = -274.47 cm⁻¹)

C	-4.74181200	0.67082500	-0.92662600
C	-3.68995900	0.94431900	-1.68480600
H	-3.50717700	1.88453100	-2.17342700
C	-2.84404400	-0.27820000	-1.81271200
C	-3.48524100	-1.19095600	-0.78400100
O	-4.73917100	-0.63200700	-0.46016200
C	-5.90663700	1.47032300	-0.50857500
H	-5.84615800	2.47041100	-0.92424100
O	-3.64388900	-2.46899500	-1.25260000
H	-6.82989400	1.00309300	-0.84717200
C	-1.14064500	2.01352100	0.98525700
C	-0.65944500	2.57405300	-0.14563600
C	1.03165000	2.17975500	1.17959500
N	-0.06695300	1.78919700	1.80562700
H	-2.14398200	1.76644800	1.27414000
H	-1.15656500	2.91501100	-1.03291700
H	2.02908200	2.12046300	1.57030100
N	0.69760500	2.67330800	0.00190800
C	-0.09424500	1.08295700	3.07676600
C	-0.23411200	-0.41619600	2.91940200
H	-0.93231400	1.46983700	3.64630400
H	0.81993400	1.33614700	3.60409200
C	0.95939300	-1.11929200	2.28474600
H	-1.15645400	-0.64361600	2.38837400
H	-0.35996100	-0.82020500	3.92009400
H	1.86404100	-0.51288500	2.27446100
H	1.19467000	-2.04529100	2.80208600
C	1.62940800	3.12433700	-1.01171100
H	1.78920800	2.33146800	-1.73375500
H	1.22031400	3.99837100	-1.50353800
H	2.56746600	3.38211100	-0.53679000
S	0.72630900	-1.60600700	0.60417000
O	1.84492100	-2.45317400	0.22645100
O	-0.52138200	-2.55195100	0.64999800
O	0.41600400	-0.46156400	-0.22472800
S	4.15963800	-0.06157400	-1.01538600
O	3.19256200	0.02945600	-2.10951700

O	4.34034400	-1.63255800	-0.71756000
O	3.66905500	0.52316400	0.23553700
O	5.51181400	0.34847200	-1.37577800
H	-4.04250500	-3.00748900	-0.56216000
H	-1.79455300	-0.13015800	-1.57446300
H	-5.95394800	1.54047400	0.57670600
H	3.48558400	-1.98438000	-0.41373500
H	-2.90749300	-0.72974900	-2.80144400
O	-2.72266900	-1.16753100	0.39430700
H	-3.28206800	-1.44928700	1.12721300
H	-1.37351700	-2.05070700	0.48879300

int11'

C	-4.74181200	0.67082500	-0.92662600
C	-3.68995900	0.94431900	-1.68480600
H	-3.50717700	1.88453100	-2.17342700
C	-2.84404400	-0.27820000	-1.81271200
C	-3.48524100	-1.19095600	-0.78400100
O	-4.73917100	-0.63200700	-0.46016200
C	-5.90663700	1.47032300	-0.50857500
H	-5.84615800	2.47041100	-0.92424100
O	-3.64388900	-2.46899500	-1.25260000
H	-6.82989400	1.00309300	-0.84717200
C	-1.14064500	2.01352100	0.98525700
C	-0.65944500	2.57405300	-0.14563600
C	1.03165000	2.17975500	1.17959500
N	-0.06695300	1.78919700	1.80562700
H	-2.14398200	1.76644800	1.27414000
H	-1.15656500	2.91501100	-1.03291700
H	2.02908200	2.12046300	1.57030100
N	0.69760500	2.67330800	0.00190800
C	-0.09424500	1.08295700	3.07676600
C	-0.23411200	-0.41619600	2.91940200
H	-0.93231400	1.46983700	3.64630400
H	0.81993400	1.33614700	3.60409200
C	0.95939300	-1.11929200	2.28474600
H	-1.15645400	-0.64361600	2.38837400
H	-0.35996100	-0.82020500	3.92009400
H	1.86404100	-0.51288500	2.27446100
H	1.19467000	-2.04529100	2.80208600
C	1.62940800	3.12433700	-1.01171100
H	1.78920800	2.33146800	-1.73375500
H	1.22031400	3.99837100	-1.50353800
H	2.56746600	3.38211100	-0.53679000

S	0.72630900	-1.60600700	0.60417000
O	1.84492100	-2.45317400	0.22645100
O	-0.52138200	-2.55195100	0.64999800
O	0.41600400	-0.46156400	-0.22472800
S	4.15963800	-0.06157400	-1.01538600
O	3.19256200	0.02945600	-2.10951700
O	4.34034400	-1.63255800	-0.71756000
O	3.66905500	0.52316400	0.23553700
O	5.51181400	0.34847200	-1.37577800
H	-4.04250500	-3.00748900	-0.56216000
H	-1.79455300	-0.13015800	-1.57446300
H	-5.95394800	1.54047400	0.57670600
H	3.48558400	-1.98438000	-0.41373500
H	-2.90749300	-0.72974900	-2.80144400
O	-2.72266900	-1.16753100	0.39430700
H	-3.28206800	-1.44928700	1.12721300
H	-1.37351700	-2.05070700	0.48879300

int12'

C	2.67279300	-1.95025200	1.38288300
C	1.46434200	-2.36807900	0.96523300
H	0.63392500	-2.63412800	1.59366800
C	1.47930700	-2.36232900	-0.47337100
C	2.72757200	-1.95280500	-0.80479100
O	3.46282600	-1.69835800	0.28119300
C	3.29381800	-1.71570200	2.69736200
H	2.57479100	-1.93716500	3.47960500
O	3.30257100	-1.79700400	-1.98876700
H	4.16535500	-2.35188800	2.84337700
C	0.99790000	2.13996300	1.84794400
C	0.57706500	1.11515700	2.61966400
C	-1.18471400	2.05802600	1.73467500
N	-0.12010500	2.72268700	1.31386200
H	1.98373600	2.50435000	1.63541100
H	1.12033200	0.42144300	3.23134200
H	-2.20335800	2.28702100	1.48576700
N	-0.78995200	1.09067600	2.54292100
C	-0.13107000	3.79279400	0.32894000
C	0.28966800	3.31357800	-1.04431200
H	0.54841100	4.56353300	0.67637500
H	-1.13467400	4.20473100	0.31254500
C	-0.70349700	2.35481200	-1.69388600
H	1.28086000	2.86767400	-0.98155600
H	0.38942200	4.19095400	-1.67574600

H	-1.60067600	2.17739700	-1.10200500
H	-1.02457300	2.69848300	-2.67403900
C	-1.65747700	0.15149300	3.22525800
H	-1.54982900	-0.83097900	2.78227800
H	-1.38353600	0.11839800	4.27314800
H	-2.68109900	0.48879600	3.12985300
S	-0.02774300	0.76152700	-1.99922200
O	-1.02020600	-0.07475200	-2.65408800
O	1.26047900	0.85310100	-2.66237900
O	0.18640500	0.29038200	-0.51610200
S	-3.16001800	-1.47681100	-0.09034100
O	-1.96221200	-2.15225300	0.41379400
O	-3.11632200	-1.63718200	-1.68925000
O	-3.15370700	-0.03311300	0.16030400
O	-4.40973600	-2.14036800	0.25992400
H	4.13481500	-1.32298400	-1.89566200
H	0.74630800	-0.52198400	-0.46494600
H	3.61564500	-0.68121100	2.80611000
H	-2.36574100	-1.12205400	-2.03177600
H	0.71239900	-2.68867800	-1.15188200
O	3.37783600	1.28428500	-0.66500700
H	4.13416700	0.70047500	-0.61834700
H	2.90018200	1.00096800	-1.44854800

TS_{12'-13'} (imaginary frequency = -105.72cm⁻¹)

C	5.04150700	0.46634400	-0.67415500
C	5.87489600	0.48684900	0.34822200
H	6.94354800	0.54864800	0.24495400
C	5.17388200	0.45432300	1.66270700
C	3.77779500	-0.01552800	1.35734700
O	3.71049200	0.45018900	-0.22447600
C	5.22839000	0.48960700	-2.13355500
H	6.28744200	0.53609800	-2.36290200
O	3.67431600	-1.34384500	1.32120300
H	4.80852000	-0.40467200	-2.59116700
C	-2.12679700	2.85805800	1.04673700
C	-3.42555200	2.56624200	1.27059600
C	-3.00959700	2.20444400	-0.84472200
N	-1.89175300	2.63973800	-0.28457400
H	-1.35906500	3.20868900	1.70884400
H	-4.01562700	2.61121500	2.16520000
H	-3.12843100	1.93819100	-1.87800100
N	-3.95814300	2.16670800	0.07422100
C	-0.59691800	2.74374300	-0.94329000

C	0.30613800	1.57989600	-0.58804600
H	-0.14933900	3.68199800	-0.63411000
H	-0.78381400	2.78737300	-2.01137100
C	-0.29991000	0.26756200	-1.03237000
H	0.47837900	1.57076100	0.48659500
H	1.26486000	1.74512100	-1.07505200
H	-1.24152300	0.06421500	-0.52943600
H	-0.46909300	0.24333400	-2.10686200
C	-5.32243700	1.72582200	-0.13454700
H	-5.53449400	0.89260900	0.52529500
H	-6.00203600	2.54287500	0.07960400
H	-5.43809000	1.41706800	-1.16517600
S	0.72509400	-1.12207800	-0.67348500
O	0.00843300	-2.31879000	-1.12479300
O	1.99505700	-0.92613200	-1.43072700
O	0.99000100	-1.10673100	0.78478900
S	-3.23194100	-1.92157200	0.25637400
O	-2.41347900	-1.19273300	1.22957200
O	-2.39733900	-3.24267700	-0.11322700
O	-3.40567200	-1.18800100	-1.00036600
O	-4.46884200	-2.46562300	0.80378700
H	2.74180400	-1.59995500	1.21144200
H	5.12331100	1.43831900	2.12387600
H	4.73163700	1.35332900	-2.57107300
H	-1.52383600	-2.96826400	-0.45322200
H	5.62189800	-0.23565000	2.37210900
O	2.80329800	0.66064800	1.95406800
H	1.94838700	0.23740500	1.76911700
H	3.05586800	-0.13000700	-0.77059700

int13'

C	5.50120700	0.11756100	-0.49644300
C	5.59147500	0.31911700	0.81528100
H	6.42462600	-0.11094900	1.34607200
C	4.57840400	1.10069300	1.57637000
C	3.26327100	0.41178900	1.74934300
O	4.43764700	0.63809400	-1.16783900
C	6.47724700	-0.64261100	-1.31512100
H	7.28357900	-1.02931400	-0.70134700
O	2.96749000	-0.64591100	1.22153100
H	5.98629600	-1.47640800	-1.81603200
C	-1.45488900	3.07976700	0.52461800
C	-2.77929600	3.06840700	0.78581500
C	-2.48238600	2.24553200	-1.21709100

N	-1.29228100	2.57548600	-0.73831700
H	-0.62183800	3.40876900	1.11509700
H	-3.33108300	3.38566400	1.64929600
H	-2.67031000	1.82098900	-2.18534900
N	-3.40129800	2.54888100	-0.31786300
C	-0.01869300	2.28943200	-1.38462700
C	0.60020800	1.00176400	-0.87766700
H	0.64175100	3.12680500	-1.18953700
H	-0.20486100	2.24160700	-2.45280300
C	-0.30930000	-0.17603700	-1.15238800
H	0.79870800	1.08688000	0.18897100
H	1.55440700	0.87852500	-1.38533800
H	-1.24716700	-0.11431100	-0.60621500
H	-0.53179700	-0.27593400	-2.21369000
C	-4.82135900	2.28683400	-0.44553100
H	-5.11637600	1.54424000	0.28722500
H	-5.37355400	3.20503800	-0.28340300
H	-5.01736700	1.91589600	-1.44315100
S	0.38967500	-1.72420800	-0.68813700
O	-0.62351000	-2.75132000	-0.86521300
O	1.65696700	-1.91012500	-1.36502100
O	0.63142300	-1.60882200	0.85030100
S	-3.57227200	-1.52735500	0.50795300
O	-2.55266300	-0.90053300	1.35263300
O	-3.12739600	-3.06702900	0.36472700
O	-3.59502400	-0.98643800	-0.85319800
O	-4.88601700	-1.62954200	1.13049100
H	1.54049100	-1.22173400	1.06195200
H	4.33729200	2.04343200	1.07945300
H	6.90204900	-0.00291600	-2.08861600
H	-2.23421900	-3.08393800	-0.02051500
H	4.93444600	1.37167000	2.56752700
O	2.43259500	1.08216300	2.51972400
H	1.59181600	0.61348600	2.58993600
H	4.52229500	0.44914400	-2.10375400

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M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, *Gaussian 09, Revision B.01*, Gaussian, Inc., Wallingford, CT, 2010.