

Supplementary information for
Study on Heterogeneous OH Oxidation of 3-Methyltetraol Sulfate in the
Atmosphere under High NO Conditions

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Table S1. The relative Gibbs energy ΔG (kcal/mol) at M06-2X/6-311++G(d,p) and DLPNO-CCSD(T)/cc-pVTZ level of theory

Reaction	ΔG_{ts-R}	ΔG_{ts-R}	ΔG_{im-R}	ΔG_{im-R}
	(M06-2X)	(DLPNO-CCSD)	(M06-2X)	(DLPNO-CCSD)
R+OH \rightarrow 1-ts1-1 \rightarrow 1-im1+H ₂ O	1.02	4.61	-31.02	-22.96
R+OH \rightarrow 1-ts1-2 \rightarrow 1-im1+H ₂ O	2.31	5.99	-31.02	-22.96
R+OH \rightarrow 1-ts1-1 \rightarrow 2-im1+H ₂ O	3.00	6.63	-25.27	-16.22
R+OH \rightarrow 2-ts1-2 \rightarrow 2-im1+H ₂ O	4.02	7.24	-25.27	-16.22
R+OH \rightarrow 2-ts1-3 \rightarrow 2-im1+H ₂ O	5.33	11.27	-25.27	-16.22
R+OH \rightarrow 3-ts1 \rightarrow 3-im1+H ₂ O	0.99	3.09	-33.40	-25.44
R+OH \rightarrow 4-ts1-1 \rightarrow 4-im1+H ₂ O	3.19	5.89	-28.45	-21.22
R+OH \rightarrow 4-ts1-2 \rightarrow 4-im1+H ₂ O	3.44	5.67	-28.45	-21.22
1-im1+O ₂ \rightarrow 1-im2	-	-	-26.13	-20.34
1-im2+NO \rightarrow 1-im3	-	-	-6.91	-5.70
1-im3 \rightarrow 1-ts2 \rightarrow 1-im4+NO ₂ +HCOOH	25.20	25.32	-25.54	-34.57
1-im4+O ₂ \rightarrow 1-im5	-	-	-26.78	-21.21
1-im5+NO \rightarrow 1-im6	-	-	-6.77	-5.01
1-im6 \rightarrow 1-ts3 \rightarrow 1-im7+NO ₂ +CH ₃ COOH	25.74	27.03	-28.53	-36.69
1-im7 \rightarrow 1-ts4 \rightarrow 1-im8+HSO ₄ ⁻	8.24	15.79	-10.49	-10.46
1-im8+H ₂ O \rightarrow 1-ts5 \rightarrow CH ₃ CHO+OH	33.45	37.57	25.52	19.00
3-im1+O ₂ \rightarrow 3-im2	-	-	-23.77	-19.84
3-im2+NO \rightarrow 3-im3	-	-	-6.29	-3.91
3-im3 \rightarrow 3-ts2 \rightarrow 3-im4+P2+NO ₂	31.07	31.43	-21.51	-29.71
3-im4+O ₂ \rightarrow 3-im5	-	-	-28.15	-20.24
3-im5+NO \rightarrow 3-im6	-	-	-8.90	-6.26
3-im6 \rightarrow 3-ts3 \rightarrow 3-im7+NO ₂	37.05	37.91	-11.98	-19.05
3-im7 \rightarrow 3-ts4 \rightarrow 3-im8+HSO ₄ ⁻	16.76	14.10	-3.65	-7.26
3-im8+H ₂ O \rightarrow 3-ts5 \rightarrow HCHO+OH	36.00	36.13	28.56	26.36

Table S2. Cartesian coordinates for all the optimized structures of reactants, transition states and products

3-MTS

C	3.14913900	0.89300300	-0.29342100
H	3.01233900	1.71165800	0.41645900
H	2.96591400	1.25799000	-1.30973100
C	2.17406800	-0.24174300	0.01758600
C	0.75176200	0.21379100	-0.34073800
H	0.72578000	0.36467400	-1.42768700
C	2.29916500	-0.69050700	1.46985000
H	1.98437500	0.10680400	2.14636900
H	1.68507000	-1.57422800	1.65393000
H	3.33750300	-0.94427500	1.69273800
O	4.46780500	0.35924000	-0.19265000
H	5.08944000	1.02872900	-0.49615300
O	2.44848600	-1.33302000	-0.86359200
H	3.39026000	-1.53197200	-0.78298300
O	0.50554400	1.44259400	0.32674500
H	-0.45114900	1.61124800	0.32302600
O	-1.49281300	-0.63881200	-0.75573200
S	-2.76139000	0.05157700	-0.00529700
O	-3.07708000	-0.80439400	1.14252700
O	-3.77235300	0.06296100	-1.05956200
O	-2.29123600	1.39433300	0.39182300
C	-0.28013400	-0.84753200	0.00647000
H	-0.50600500	-0.84632900	1.07580500
H	0.07788900	-1.83482000	-0.28195200

1-ts-1

C	3.01236000	0.18207400	-0.67015600
H	2.95982500	1.27466000	-0.31191100
H	2.83864600	0.18972000	-1.74811900
C	1.93697200	-0.64186400	0.05180700
C	0.55236400	-0.21434800	-0.46114200
H	0.51867800	-0.45021600	-1.53210100
C	2.06414400	-0.53501600	1.56652600
H	1.86153600	0.48429700	1.90105400
H	1.36474900	-1.21654200	2.05416700
H	3.07158700	-0.81417300	1.88751700
O	4.31443700	-0.29889400	-0.45482100
H	4.53611800	-0.21641600	0.48130600

O	2.07908200	-1.99835000	-0.36922200
H	2.98122700	-2.27691300	-0.16554700
O	0.41603400	1.18816200	-0.27399100
H	-0.52845000	1.42129500	-0.24872000
O	-1.77813300	-0.87256800	-0.55989700
S	-2.95421800	0.10566200	-0.00099900
O	-3.32686500	-0.40942300	1.31984700
O	-3.98297700	-0.03091000	-1.02773200
O	-2.33553900	1.44563000	0.05883200
C	-0.56558300	-0.98536000	0.22128400
H	-0.73638500	-0.61795500	1.23645300
H	-0.33042100	-2.04769900	0.25974000
O	2.73335400	2.63892000	0.26723300
H	1.77369500	2.44589700	0.27024100
1-ts-2			
C	2.94474000	0.11240500	0.79435200
H	2.72121100	-0.08518600	1.84184900
H	2.87709400	1.25681600	0.64162100
C	1.92083800	-0.50942100	-0.16059800
C	0.54721200	0.13159700	0.09471300
H	0.62257600	1.18346700	-0.21087000
C	1.90372000	-2.02545700	-0.01699600
H	1.53958400	-2.30729100	0.97246600
H	1.25841900	-2.47589800	-0.77421500
H	2.91289300	-2.42340100	-0.14243100
O	4.26238100	-0.29479700	0.54566400
H	4.46637700	-0.12520300	-0.38403600
O	2.27714900	-0.12442000	-1.49258000
H	2.82868700	-0.81178900	-1.88544400
O	0.27980300	0.04524300	1.48552200
H	-0.66694800	0.21045100	1.62943900
O	-1.66787500	0.37720700	-0.88324100
S	-2.98026000	0.10361500	0.03828600
O	-3.43981500	-1.24976800	-0.28954600
O	-3.88019000	1.17475300	-0.38322400
O	-2.50728000	0.22788000	1.43204100
C	-0.53970500	-0.51817000	-0.74583000
H	-0.86448300	-1.46700100	-0.31071600
H	-0.18298900	-0.69276700	-1.75975100
O	3.01390500	2.46762300	-0.28262200
H	2.80629300	1.94447500	-1.08043100
2-ts-1			
C	3.00367000	-0.18010300	-0.99372800
H	2.94203500	0.86400900	-1.30581500

H	2.73376700	-0.82322100	-1.83413800
C	2.04206800	-0.45091000	0.16910900
C	0.59795300	-0.43864700	-0.35608800
H	0.49424700	-1.31361600	-1.00900400
C	2.28114400	0.51171400	1.32372900
H	2.00662200	1.61010600	1.00267600
H	1.66379500	0.29317400	2.19545900
H	3.33478100	0.56474100	1.60615900
O	4.33784100	-0.52031300	-0.63221100
H	4.72419400	0.21203800	-0.13923300
O	2.25843100	-1.78112900	0.64007900
H	3.21472600	-1.89163100	0.73555100
O	0.41493400	0.75051300	-1.11699400
H	-0.53328100	0.84142300	-1.32028500
O	-1.66957900	-1.09260100	0.29651800
S	-2.86268800	-0.04579800	-0.06583600
O	-3.10702000	0.73673500	1.14949700
O	-3.94920800	-0.94302100	-0.45034500
O	-2.33936600	0.77207800	-1.17902900
C	-0.41115300	-0.56715300	0.77544500
H	-0.56917800	0.39315600	1.27477700
H	-0.06218900	-1.29597000	1.50618700
O	1.52418000	2.79432100	0.42691000
H	1.00968200	2.29648100	-0.24515300
2-ts-2			
C	-2.73247900	-1.07511000	0.63170000
H	-2.72459100	-0.66765800	1.64540200
H	-2.37464500	-2.10636700	0.65717000
C	-1.81170500	-0.24297700	-0.27863000
C	-0.34887900	-0.61958400	0.02205400
H	-0.23321000	-1.67300200	-0.26392200
C	-2.03811000	1.24801800	-0.09444100
H	-1.69192600	1.60822000	0.87474600
H	-1.62834700	1.84436300	-0.91172900
H	-3.18262100	1.46493500	-0.12621000
O	-4.05394100	-1.11744300	0.11096100
H	-4.45771900	-0.24336100	0.23653300
O	-2.04428800	-0.62082400	-1.63062600
H	-2.99331700	-0.79116400	-1.71160700
O	-0.14011600	-0.46484600	1.41601500
H	0.81410300	-0.39435300	1.58649300
O	1.91050200	-0.45941000	-0.85515100
S	3.11101900	0.13548200	0.06864000
O	3.30853200	1.52467800	-0.35724000

O	4.21632400	-0.76630000	-0.24602200
O	2.61886500	0.02401200	1.45688900
C	0.62412200	0.20079200	-0.80817400
H	0.73343600	1.21266300	-0.40851000
H	0.28545800	0.25980300	-1.84165900
O	-4.57591800	1.65929600	0.25365600
H	-4.40029800	2.01807800	1.14214200
2-ts-3			
C	2.99617500	-1.36359500	-0.17528800
H	2.84031700	-1.70288700	-1.19861700
H	2.73859100	-2.17573200	0.51382400
C	2.08946800	-0.15603800	0.13147400
C	0.64377900	-0.65712300	0.26060400
H	0.60871200	-1.29129800	1.15620700
C	2.26597600	0.90036300	-0.94178600
H	1.75357100	0.64708800	-1.87007600
H	1.82624800	1.91521200	-0.57016900
H	3.31799800	1.12440600	-1.12810400
O	4.36971000	-1.03027900	-0.05685700
H	4.55520400	-0.85192400	0.87258400
O	2.42964700	0.35255900	1.42071800
H	3.17398100	0.95997500	1.33207600
O	0.34903100	-1.42930600	-0.89325300
H	-0.61501600	-1.47538200	-1.00543000
O	-1.58370800	-0.04112000	0.98992100
S	-2.86150900	-0.13897800	-0.01295300
O	-3.12411800	1.22521000	-0.48215900
O	-3.89353500	-0.69767000	0.85681800
O	-2.42821800	-1.04548700	-1.09545900
C	-0.34309200	0.47962300	0.45754400
H	-0.52905800	1.00676500	-0.48272100
H	0.02936500	1.18506200	1.19843200
O	1.34460300	3.23619000	-0.28138700
H	0.46310400	3.10219500	-0.67276800
3-ts-1			
C	3.06652200	-0.11150300	0.91380100
H	2.89282700	-0.86506400	1.68504700
H	2.92106300	0.88658600	1.34027400
C	2.09088400	-0.31068200	-0.24611200
C	0.67859800	0.06810200	0.21709300
H	0.71119500	1.20290200	0.40511400
C	2.14986600	-1.73700900	-0.78409600
H	1.78335700	-2.44268000	-0.03568700
H	1.54484400	-1.82872400	-1.68805700

H	3.18126900	-1.99477900	-1.03250900
O	4.38186200	-0.23349100	0.37946500
H	5.01012100	0.03920500	1.05595200
O	2.41244000	0.62251000	-1.28080500
H	3.35892000	0.53712100	-1.45747700
O	0.39277700	-0.58907900	1.41962500
H	-0.57334900	-0.63897900	1.53897500
O	-1.54414100	0.66283100	-0.54755900
S	-2.85244100	-0.10523000	0.04906200
O	-3.27063500	-1.06603000	-0.97505500
O	-3.77826200	1.00111000	0.27251400
O	-2.37556900	-0.75595000	1.28658500
C	-0.37899700	-0.13006800	-0.85572600
H	-0.64924500	-1.18623700	-0.94576900
H	-0.01107600	0.23076700	-1.81497100
O	1.04437900	2.69036900	0.10003300
H	1.72508400	2.41236900	-0.54405400
4-ts-1			
C	3.05901600	-0.87196900	-0.67013800
H	2.95358400	-0.58200100	-1.71752500
H	2.76713400	-1.92039200	-0.55118000
C	2.17059500	0.00192600	0.21562100
C	0.70236700	-0.37365000	-0.02856100
H	0.57749000	-1.42186100	0.27260500
C	2.44546200	1.48343700	-0.02405100
H	2.16729400	1.76919300	-1.04083800
H	1.88480800	2.09895800	0.68257600
H	3.50890600	1.68789200	0.11594000
O	4.40346400	-0.68335100	-0.23223800
H	4.94297300	-1.39132000	-0.59811800
O	2.42160600	-0.33200800	1.58146200
H	3.38074000	-0.32149100	1.69908900
O	0.43638100	-0.22806500	-1.41322200
H	-0.36817600	-0.73429500	-1.60238000
O	-1.47910700	-0.11760800	1.15615600
S	-2.58456500	-0.42847800	-0.01556000
O	-2.78815200	0.84760400	-0.71436000
O	-3.72142600	-0.88636400	0.77148400
O	-1.98719700	-1.46255500	-0.87494900
C	-0.22271900	0.46599200	0.84728600
H	-0.38279000	1.49831700	0.32823500
H	0.22394800	0.68988500	1.81542700
O	-0.74252400	2.72594600	-0.33927700
H	-1.57556000	2.33955900	-0.67625400

4-ts-2

C	-3.09495600	-1.16416300	-0.35511700
H	-2.88520500	-2.07072700	0.21618100
H	-2.96340500	-1.36790900	-1.42271600
C	-2.14447200	-0.04273500	0.06450500
C	-0.73151700	-0.37382200	-0.43923200
H	-0.74188000	-0.28892800	-1.53250500
C	-2.19382500	0.18816600	1.57028400
H	-1.77745100	-0.67160700	2.09999800
H	-1.62621700	1.08116700	1.84075400
H	-3.22694700	0.32865700	1.89339100
O	-4.42066200	-0.70559600	-0.10007500
H	-5.03633200	-1.28799800	-0.55630300
O	-2.53133000	1.14679900	-0.63498800
H	-3.47904000	1.26799400	-0.48599800
O	-0.43332000	-1.70875300	-0.05403800
H	0.52911900	-1.83702100	-0.04679300
O	1.51412500	0.45124800	-0.68774300
S	2.83883300	-0.21518600	0.02744900
O	3.13124700	0.62120500	1.19204900
O	3.82240300	-0.15193900	-1.04699100
O	2.40081300	-1.57745500	0.37971300
C	0.33628500	0.56538500	0.09579000
H	0.53912100	0.41543400	1.15977100
H	0.00402800	1.67743300	-0.00786000
O	-0.52925900	2.99144900	-0.15575600
H	-1.41835500	2.62383800	-0.35184800

1-im-1

C	3.15738000	0.83722100	-0.38377900
H	2.97781000	1.44990600	-1.26202900
C	2.20898600	-0.25833800	-0.02199100
C	0.78114400	0.20932400	-0.35134200
H	0.73619600	0.36854800	-1.43678900
C	2.36975300	-0.68853300	1.43305600
H	2.11829000	0.13284100	2.10644700
H	1.72455600	-1.54148400	1.65208200
H	3.40349600	-0.98553100	1.62118700
O	4.46708300	0.58871100	-0.06112900
H	5.03452400	1.23161500	-0.50220200
O	2.42429800	-1.39652200	-0.88784800
H	3.31172400	-1.73144100	-0.70994700
O	0.55335400	1.43295900	0.33058800
H	-0.40216300	1.61016300	0.33407900
O	-1.46923800	-0.63580600	-0.74813600

S	-2.72804400	0.06668500	0.00705800
O	-3.04513800	-0.78456100	1.15815500
O	-3.74419600	0.08407200	-1.04226300
O	-2.24509900	1.40626300	0.39931100
C	-0.25241100	-0.84736500	0.00677000
H	-0.47110400	-0.83883600	1.07761400
H	0.09774300	-1.83752000	-0.27909000
1-im-2			
C	3.16741700	0.86130800	-0.33076400
H	2.96405200	1.89098100	-0.06349600
C	2.20700600	-0.23877200	0.01155300
C	0.78308300	0.21152000	-0.35469900
H	0.75706200	0.34345700	-1.44398700
C	2.33194500	-0.64371500	1.48335300
H	2.03822100	0.18287000	2.13296700
H	1.70452800	-1.51107400	1.70183300
H	3.36989400	-0.90512700	1.70226700
O	4.47957900	0.45924600	-0.30786900
H	5.05587100	1.22972000	-0.37134800
O	2.46735400	-1.37257800	-0.82497900
H	3.34992200	-1.69970600	-0.61203300
O	0.53976200	1.45069700	0.29287500
H	-0.41777800	1.61489800	0.30011500
O	-1.46180500	-0.63953100	-0.75192300
S	-2.73093000	0.05560400	-0.00681600
O	-3.05407200	-0.79880600	1.14015500
O	-3.73782800	0.07000100	-1.06491000
O	-2.25692200	1.39672100	0.39150100
C	-0.25013200	-0.84155700	0.01356000
H	-0.47546600	-0.81949000	1.08281100
H	0.10411000	-1.83488100	-0.25688500
2-im-1			
C	3.19682900	0.84560000	-0.32237600
H	3.02403700	1.73636100	0.28545600
H	3.07691400	1.09576900	-1.38113600
C	2.19579200	-0.24947100	0.04859800
C	0.78139600	0.19442900	-0.38603900
H	0.78830100	0.27166500	-1.48077300
C	2.26965000	-0.56394200	1.50721400
H	2.07137500	-1.57241600	1.84741800
H	2.40117600	0.22822100	2.23243900
O	4.49799400	0.31558100	-0.08131000
H	5.14320300	0.88665500	-0.51086500
O	2.47310600	-1.41257800	-0.73224400

H	3.40875100	-1.61799000	-0.60553500
O	0.52755800	1.46339100	0.19401500
H	-0.43242800	1.61190300	0.21962600
O	-1.47224900	-0.64198200	-0.74482000
S	-2.74045200	0.04742400	0.00873700
O	-3.05441600	-0.81050900	1.15535200
O	-3.75261100	0.06121700	-1.04413100
O	-2.26627100	1.38853500	0.40697600
C	-0.25695500	-0.83958500	0.01430300
H	-0.46689200	-0.78800300	1.08626300
H	0.08763400	-1.84236800	-0.23359700

2-im-2

C	3.19681400	0.84559700	-0.32239200
H	3.02401800	1.73636600	0.28542500
H	3.07689300	1.09574700	-1.38115600
C	2.19577700	-0.24947300	0.04860000
C	0.78138400	0.19442800	-0.38603900
H	0.78828700	0.27167000	-1.48077300
C	2.26962500	-0.56391300	1.50722300
H	2.40093900	0.22829300	2.23243900
H	2.07161800	-1.57243600	1.84743300
O	4.49797900	0.31558200	-0.08132100
H	5.14318900	0.88666300	-0.51086400
O	2.47309700	-1.41259100	-0.73222000
H	3.40874900	-1.61797900	-0.60552800
O	0.52755400	1.46338800	0.19402200
H	-0.43243700	1.61189100	0.21965200
O	-1.47225900	-0.64201000	-0.74481900
S	-2.74043700	0.04742900	0.00873900
O	-3.05443300	-0.81051700	1.15533800
O	-3.75258200	0.06125600	-1.04414400
O	-2.26621100	1.38852100	0.40698700
C	-0.25696100	-0.83959400	0.01430100
H	-0.46690000	-0.78800800	1.08626200
H	0.08763400	-1.84237600	-0.23359500

2-im-3

C	3.19682900	0.84560400	-0.32236700
H	3.02403900	1.73634800	0.28549000
H	3.07690200	1.09579900	-1.38111900
C	2.19580400	-0.24947700	0.04859100
C	0.78140200	0.19442100	-0.38603100
H	0.78830000	0.27165100	-1.48076500
C	2.26968400	-0.56399000	1.50719700
H	2.40142900	0.22812200	2.23243700

H	2.07116600	-1.57242200	1.84738900
O	4.49799600	0.31558600	-0.08132700
H	5.14321900	0.88684100	-0.51062700
O	2.47310900	-1.41256700	-0.73228600
H	3.40873900	-1.61802800	-0.60554400
O	0.52756700	1.46338800	0.19401600
H	-0.43241400	1.61190800	0.21963200
O	-1.47224200	-0.64198500	-0.74480400
S	-2.74046300	0.04742500	0.00873500
O	-3.05441000	-0.81046600	1.15538200
O	-3.75262900	0.06117400	-1.04412400
O	-2.26630700	1.38855600	0.40693300
C	-0.25695300	-0.83958300	0.01432600
H	-0.46689000	-0.78798600	1.08628500
H	0.08763800	-1.84236900	-0.23355800

3-im-1

C	3.01218600	0.96337700	-0.36272000
H	2.97962800	1.72191300	0.42311700
H	2.59957400	1.38010800	-1.28690200
C	2.18430600	-0.25520600	0.04700900
C	0.73320900	0.12472700	0.14275700
C	2.68436300	-0.84009500	1.37289300
H	2.57739300	-0.10260400	2.17177000
H	2.10152100	-1.72738600	1.63009700
H	3.73696900	-1.12232100	1.29458900
O	4.34820400	0.51559700	-0.57317100
H	4.85038800	1.23796700	-0.96395300
O	2.27003400	-1.24308900	-0.98336700
H	3.20528800	-1.45829400	-1.09186700
O	0.51114900	1.33390800	0.73872100
H	-0.45325600	1.48008300	0.80213300
O	-1.41708000	-0.66365400	-0.69728000
S	-2.73189700	0.07828000	-0.09814700
O	-3.33174000	-0.84853700	0.86708500
O	-3.53393500	0.31616200	-1.29602400
O	-2.22187900	1.31114900	0.54067600
C	-0.31925900	-0.91827800	0.23686200
H	-0.73544900	-0.99406200	1.24867900
H	0.08142800	-1.88730900	-0.05123700

4-im-1

C	3.18825600	0.81483700	-0.39204300
H	3.09973700	1.70230900	0.23926400
H	3.00100400	1.09044900	-1.43496000
C	2.17137700	-0.24183200	0.03609400

C	0.76314500	0.26068500	-0.30974500
H	0.72526400	0.43275100	-1.39225400
C	2.33127000	-0.58934400	1.51203900
H	2.09713200	0.27310900	2.13889300
H	1.67622800	-1.41766700	1.78637900
H	3.36165400	-0.89164700	1.70971100
O	4.48513200	0.23610900	-0.26262500
H	5.11587300	0.80037700	-0.72089600
O	2.35281500	-1.40655900	-0.77087700
H	3.29085800	-1.63565200	-0.72986600
O	0.56273100	1.50449800	0.37726600
H	-0.38658700	1.70274200	0.35530600
O	-1.44888000	-0.66048100	-0.73333800
S	-2.78828100	0.02436200	-0.01528200
O	-3.08551400	-0.82025700	1.14147300
O	-3.76629700	-0.03046700	-1.09488200
O	-2.33737100	1.37856600	0.34361300
C	-0.29909700	-0.72276300	0.03363100
H	-0.39929300	-1.18732500	1.00803100
4-im-2			
C	3.18826200	0.81483900	-0.39203000
H	3.09971900	1.70231200	0.23927100
H	3.00103400	1.09044600	-1.43495300
C	2.17137800	-0.24183400	0.03608500
C	0.76315100	0.26068800	-0.30976400
H	0.72527900	0.43276100	-1.39227200
C	2.33126000	-0.58936300	1.51202700
H	2.09713300	0.27308400	2.13889200
H	1.67620300	-1.41767900	1.78635600
H	3.36163900	-0.89168700	1.70969800
O	4.48514000	0.23612300	-0.26257900
H	5.11587500	0.80035500	-0.72090400
O	2.35282100	-1.40655100	-0.77089800
H	3.29085200	-1.63568000	-0.72983500
O	0.56273000	1.50449700	0.37725100
H	-0.38659100	1.70272300	0.35532100
O	-1.44888200	-0.66044500	-0.73336400
S	-2.78828400	0.02436000	-0.01527400
O	-3.08549900	-0.82030000	1.14145500
O	-3.76630700	-0.03043900	-1.09486700
O	-2.33738100	1.37855600	0.34366500
C	-0.29909600	-0.72275900	0.03360000
H	-0.39929700	-1.18733200	1.00799300

1-im2

C	1.66592300	-0.77602900	0.05295200
C	0.31778800	-0.17926700	-0.38466100
H	0.29181300	-0.22645400	-1.48095700
C	1.76980200	-0.99166300	1.55825300
H	1.52505700	-0.07938300	2.10389000
H	1.07894100	-1.78071800	1.85966100
H	2.78240400	-1.30101800	1.82699900
O	3.99844800	-0.61849200	-0.42111900
H	4.63364900	-0.23268200	-1.03759400
O	1.75267400	-2.00819600	-0.64904400
H	2.60579600	-2.41212800	-0.44387800
O	0.26187700	1.16847500	0.04732100
H	-0.66713400	1.45497600	0.05816300
O	-2.02864600	-0.74327500	-0.64909500
S	-3.17579700	0.22516900	-0.01899600
O	-3.62000000	-0.41471100	1.22269300
O	-4.17245300	0.25346400	-1.08604300
O	-2.50045000	1.51822000	0.21215000
C	-0.84683800	-1.00336000	0.14267200
H	-1.04215100	-0.78341200	1.19557900
H	-0.64591600	-2.06746500	0.02998100
C	2.81903900	0.10392800	-0.46904300
H	2.62052800	0.51085500	-1.46262100
O	2.95500800	1.25681100	0.42663100
O	3.76297800	2.13683700	-0.07178300
1-im3			
C	-0.92435900	1.12689400	0.06724400
C	0.32596300	0.36778100	-0.41024900
H	0.34993000	0.45634800	-1.50397300
C	-1.00562500	1.26374500	1.58295500
H	-0.92197100	0.29142200	2.07087600
H	-0.19623600	1.90701900	1.93259600
H	-1.95580700	1.71992300	1.86985100
O	-3.25243400	1.39206200	-0.44877400
H	-3.79496200	1.31177200	-1.24198900
O	-0.81878100	2.40157000	-0.55201000
H	-1.64911500	2.87153400	-0.39762900
O	0.21611000	-0.99327000	-0.03432000
H	1.10358000	-1.38904200	-0.02082700
O	2.72632300	0.57114400	-0.65569000
S	3.74495500	-0.51993300	-0.00266100
O	4.24745700	0.07578100	1.23870100
O	4.74304500	-0.67549600	-1.05705300
O	2.91777800	-1.72115700	0.22811900

C	1.59529900	1.00505500	0.13420900
H	1.74761100	0.74521200	1.18506500
H	1.55818600	2.08836600	0.03408700
C	-2.20347200	0.47170400	-0.50911000
H	-2.04668800	0.12464200	-1.53308400
O	-2.51114700	-0.65031100	0.31790300
O	-3.56386800	-1.34556300	-0.28782800
N	-4.75764700	-1.00654700	0.41692800
O	-5.64662100	-1.57644900	-0.05669600

l-im4

C	2.78021200	0.03687400	-0.15096300
C	1.37400700	0.08363500	-0.66423000
H	1.34361600	-0.44144600	-1.62734700
C	3.15269300	0.63494400	1.16114500
H	2.65101200	1.59375400	1.29837900
H	2.87065100	-0.02232800	1.99712900
H	4.23266400	0.79854600	1.21955900
O	3.40934700	-1.13629200	-0.51806100
H	4.23653100	-1.22597500	-0.02885000
O	1.00106300	1.44576600	-0.83195000
H	0.03399600	1.51967300	-0.77544300
O	-0.83061100	-0.92836700	-0.33895800
S	-2.11746000	-0.02953700	0.09402600
O	-2.28037600	-0.20942900	1.53937000
O	-3.18323300	-0.60881900	-0.72016000
O	-1.75855700	1.35378500	-0.27694700
C	0.44141000	-0.65183700	0.29275000
H	0.29486000	-0.07888800	1.21280100
H	0.86503100	-1.62558500	0.54079000

l-im5

C	0.80436500	0.19503200	-0.36550800
H	0.79737100	0.32475100	-1.45478800
C	2.42225500	-0.55715300	1.48574300
H	2.13969700	0.30883200	2.08353600
H	1.81627000	-1.41594800	1.77923400
H	3.47391000	-0.79241900	1.66081900
O	2.54371800	-1.33151100	-0.80895000
H	3.31201700	-1.79153900	-0.44565000
O	0.57580400	1.42870800	0.28670500
H	-0.38221000	1.59432900	0.31251200
O	-1.43676400	-0.65381600	-0.75652000
S	-2.69695100	0.04925500	0.00464900
O	-3.00830700	-0.80461900	1.15408700
O	-3.71285600	0.06823400	-1.04339500

O	-2.20789400	1.38637800	0.39657000
C	-0.22507200	-0.86629500	-0.00393200
H	-0.43747800	-0.85604200	1.06847000
H	0.13164800	-1.85470000	-0.28962100
C	2.20648600	-0.27758100	0.01868900
O	3.06020600	0.89336900	-0.35637000
O	4.31756900	0.60458500	-0.32198500
1-im6			
C	0.18101400	0.23059200	-0.19657600
H	0.27653600	0.50889500	-1.25352600
C	1.58461100	-0.87510000	1.64614200
H	1.23018600	-0.12381200	2.35159800
H	0.94976200	-1.76043800	1.71017900
H	2.60458200	-1.16259600	1.90641200
O	1.92857300	-1.26339900	-0.72292600
H	2.52005300	-1.91470600	-0.32430800
O	-0.10925200	1.36865800	0.59188000
H	-1.07301200	1.49611000	0.61756900
O	-2.02793700	-0.46638100	-0.88732800
S	-3.35851700	0.07282400	-0.11516100
O	-3.80265100	-1.02117900	0.75325700
O	-4.25279900	0.37822800	-1.22810900
O	-2.90290300	1.25707600	0.63993800
C	-0.88963700	-0.84503500	-0.08535100
H	-1.18946900	-0.99430300	0.95546200
H	-0.53043600	-1.78784900	-0.49431100
C	1.54444600	-0.32615100	0.23717400
O	2.39920800	0.84260400	0.11817500
O	3.71354400	0.47570400	0.41455100
N	4.40148100	0.34050300	-0.82459400
O	5.50610600	0.06420700	-0.61227400
1-im7			
C	-2.40013300	0.29656600	-0.19098800
H	-3.23396600	0.63569800	-0.78742100
O	-2.38776500	-1.03924300	0.07337800
H	-1.49962500	-1.29632400	0.38703800
O	-0.06463500	0.84535000	-0.66359900
S	1.06509300	-0.10369100	0.01004000
O	1.66641400	0.67342200	1.09983300
O	1.96402900	-0.37959400	-1.10968800
O	0.33181700	-1.29137800	0.50008800
C	-1.25635100	1.14236100	0.16680200
H	-0.96384100	1.03045000	1.21601500
H	-1.48401800	2.18720900	-0.03124500

1-im8

C	0.12988500	0.40963400	0.00001800
H	0.19322700	1.50613500	0.00002600
O	1.16791400	-0.26575100	-0.00001300
C	-1.16639000	-0.17331900	-0.00000300
H	-1.26941700	-1.25163800	0.00006300
H	-2.04809900	0.45362000	-0.00007700

1-ts2

C	-0.72649500	1.26719900	0.11947800
C	0.27229000	0.31074500	-0.53848100
H	-0.00742900	0.17519600	-1.58726900
C	-0.81215800	1.24919200	1.61909800
H	-0.96846500	0.24002900	1.99322900
H	0.12889500	1.64341600	2.01432300
H	-1.62168100	1.89892300	1.95937900
O	-3.28969100	1.77429300	-0.15262500
H	-3.59562800	1.57284500	0.74508300
O	-0.59273800	2.50764800	-0.42719200
H	-1.05861200	3.16557900	0.11000800
O	0.25274200	-0.95403200	0.08019800
H	0.98845300	-1.02177500	0.71081700
O	2.62076400	0.01845600	-1.00117600
S	3.68432500	-0.60150400	0.07521300
O	4.52749000	0.51942800	0.50080100
O	4.36664500	-1.61567700	-0.72317200
O	2.85127700	-1.13886900	1.16783400
C	1.66164600	0.95650000	-0.48969500
H	1.92021200	1.25003300	0.53144800
H	1.69253800	1.83410900	-1.13081500
C	-2.38376400	0.82789200	-0.55175400
H	-2.18060100	0.92380500	-1.61967300
O	-2.44322400	-0.34025800	-0.02483600
O	-3.91189300	-1.18429800	-0.64699600
N	-4.61187900	-1.44870800	0.39841800
O	-5.63547800	-2.03497900	0.14332200

1-ts3

C	0.10629900	0.40986400	-0.75612600
H	0.51281100	0.55217800	-1.75211300
C	1.15921400	-0.09854600	1.70216600
H	0.96252200	0.95252600	1.90276700
H	0.31096500	-0.71050200	2.00712800
H	2.04148800	-0.41592700	2.26324600
O	1.63925600	-1.62250700	-0.06178400
H	2.00025600	-1.70299100	-0.95780200

O	-0.29307100	1.57828200	-0.21973300
H	-0.96344700	1.43010100	0.47921100
O	-2.16529800	-0.25658700	-1.10459400
S	-3.27231300	-0.00440000	0.08624500
O	-3.63213800	-1.33241900	0.58300900
O	-4.32644800	0.70216200	-0.62943000
O	-2.55528600	0.80885500	1.08914600
C	-0.89303600	-0.75922500	-0.68673400
H	-0.96095900	-1.19416900	0.31088400
H	-0.59502800	-1.52617500	-1.39634900
C	1.47688800	-0.29494800	0.24632600
O	2.25301300	0.54595300	-0.35277100
O	3.90740300	0.48836300	0.41179400
N	4.67089400	0.02636300	-0.51215500
O	5.82956400	-0.04235800	-0.17633700
1-ts4			
C	2.44240600	-0.11757900	-0.23226000
H	3.28709700	-0.25248500	-0.90036600
O	2.19683400	1.11026900	0.12278100
H	1.23350000	1.17501300	0.47845800
O	-0.07729300	-0.78560800	-0.86712600
S	-1.06332600	0.03102300	-0.01427300
O	-1.69127900	-0.85660500	0.98982000
O	-2.05245100	0.65030200	-0.92075000
O	-0.25296300	1.09843800	0.69142500
C	1.64754300	-1.18997800	0.17341000
H	1.11390400	-1.14118100	1.11441400
H	1.85624100	-2.16675000	-0.24024800
1-ts5			
C	-1.15890000	0.06515900	0.00001900
H	-2.21453700	0.38528000	0.00006100
O	-0.88167100	-1.11429200	-0.00001600
C	-0.15490900	1.16192500	-0.00000900
H	-0.23297200	1.77843800	0.89820200
H	-0.23284700	1.77821300	-0.89838900
O	1.91943400	-0.25361800	0.00000300
H	0.92968700	0.67109900	0.00011300
H	1.33141800	-1.03225800	0.00004900
CH3CHO			
C	0.23474800	0.39888400	-0.00002500
H	0.31789700	1.50473400	0.00002200
O	1.22597200	-0.27825600	-0.00000500
C	-1.16469500	-0.14715200	-0.00003500
H	-1.14849000	-1.23553600	-0.00020100

H	-1.69908600	0.22345200	-0.87901800
H	-1.69841600	0.22300600	0.87959800
CH ₃ COOH			
O	0.78649900	-1.02932300	0.00003800
H	1.72534200	-0.79905600	0.00006400
C	0.09031500	0.12664300	-0.00010300
O	0.62701000	1.19862700	-0.00004200
C	-1.38980900	-0.12192800	0.00005200
H	-1.66039600	-0.70608400	-0.88050300
H	-1.66022600	-0.70601600	0.88070600
H	-1.91583700	0.82844100	0.00006900
HCOOH			
O	1.11069600	-0.08913600	0.00001600
H	1.05183200	-1.05532200	-0.00010600
C	-0.13523600	0.39892300	0.00000400
H	-0.10956000	1.49502600	-0.00006900
O	-1.12705300	-0.26502000	0.00000300
HSO ₄			
H	1.98574000	0.25899200	0.00157300
O	-0.24268600	0.82601400	1.22716700
S	-0.14810300	0.02957500	-0.00018900
O	-0.23788800	0.82700100	-1.22730600
O	-0.90330300	-1.21602100	-0.00211900
O	1.43186500	-0.52851800	0.00244000
3-im ₂			
C	-3.11040800	-0.41862000	0.67982900
H	-2.93836600	-0.26959400	1.74789000
H	-2.98151600	-1.47594600	0.43417200
C	-2.12688400	0.43129400	-0.13151600
C	-2.16864600	1.88972500	0.31699300
H	-1.80710000	1.99377500	1.34149700
H	-1.56357100	2.51313200	-0.34337600
H	-3.19925800	2.24550700	0.27138600
O	-4.41740300	0.01412700	0.31492600
H	-5.04611400	-0.66272500	0.58550700
O	-2.44512800	0.32920300	-1.51377200
H	-3.40294100	0.44158500	-1.58598400
O	-0.44106000	-0.31466000	1.36001600
H	0.52477500	-0.34818400	1.51411900
O	1.54474500	-0.09335200	-0.91594200

S	2.79874800	0.20741000	0.09237400
O	3.13005000	1.62214400	-0.08137100
O	3.80466600	-0.73218400	-0.38755700
O	2.27457500	-0.10040600	1.43933100
C	0.34369100	0.66589100	-0.73739400
H	0.54540000	1.59708400	-0.20345800
H	-0.02853200	0.89304400	-1.73479100
C	-0.70628100	-0.14073400	0.03130000
O	-0.75371100	-1.47299000	-0.65640700
O	0.01931800	-2.35332900	-0.11674900
3-im3			
C	2.57826300	-1.01910000	0.93492600
H	2.16503500	-1.53318300	1.80494800
H	2.83728500	0.00132100	1.21109900
C	1.55966900	-1.05771600	-0.21956600
C	1.13053600	-2.51216800	-0.43337200
H	0.52907100	-2.86553500	0.40713800
H	0.56124000	-2.62181100	-1.35702200
H	2.02171900	-3.13698600	-0.50872500
O	3.74238500	-1.70058200	0.46526800
H	4.51081700	-1.32173400	0.90277000
O	2.16137200	-0.54480700	-1.39952500
H	3.01886400	-0.98455700	-1.48255800
O	0.02161800	-0.26680900	1.41447400
H	-0.92440700	-0.07776700	1.56416500
O	-1.88846300	0.46039800	-0.78870200
S	-3.23042600	0.10839100	0.07816500
O	-3.77919000	-1.11932200	-0.50112400
O	-4.04001600	1.30531600	-0.12216300
O	-2.74325600	-0.07238300	1.46074800
C	-0.85519200	-0.53182300	-0.85513300
H	-1.24315600	-1.50982700	-0.56779800
H	-0.51847000	-0.56348200	-1.89053500
C	0.31960700	-0.16314100	0.06216200
O	0.52220800	1.21811800	-0.30089600
O	1.59582400	1.75318400	0.42151500
N	2.54890200	2.19365700	-0.53135200
O	3.46866900	2.62031200	0.03181000
3-im4			
O	0.98915900	-0.74533000	0.15809800
S	-0.46153000	0.04348400	-0.01042300
O	-0.39624300	1.16570700	0.92834000
O	-1.39953900	-1.01249200	0.35892100
O	-0.51110800	0.44844800	-1.41702500

C	2.13077300	0.00166400	-0.04704200
H	2.11350200	1.04170800	0.25426300
H	3.02819900	-0.59809200	-0.03191800
3-im5			
O	-0.25242500	0.17202900	-0.84016600
S	1.12930800	-0.09268300	0.05399200
O	1.72241400	1.23554100	0.21589000
O	1.86009900	-0.99358000	-0.82929500
O	0.66499600	-0.68853900	1.30750900
C	-1.25727900	0.93363800	-0.23951500
H	-0.87927400	1.65593600	0.48365500
H	-1.84700000	1.39262100	-1.02916000
O	-2.13763400	0.07863900	0.52782100
O	-2.83232200	-0.70002200	-0.24191800
3-im6			
O	-0.28031400	0.25616600	0.82202000
S	-1.57435600	-0.28156500	-0.06157700
O	-2.65709700	0.65207100	0.26141100
O	-1.74480100	-1.62798200	0.47608300
O	-1.14919400	-0.22213700	-1.46234400
C	0.29435700	1.48374600	0.44083800
H	-0.41933000	2.15635100	-0.03892400
H	0.72725000	1.92026100	1.33874900
O	1.30046500	1.29314000	-0.53427600
O	2.36194900	0.61572800	0.07860900
N	2.23841800	-0.76682400	-0.27180400
O	3.09983100	-1.35527200	0.22637300
3-im7			
O	-0.50880700	0.73744600	-0.63907700
S	0.78298400	-0.06514900	0.03897600
O	1.14708500	0.71228000	1.22277900
O	1.75555900	-0.02924500	-1.04628600
O	0.24521300	-1.39838600	0.34675700
C	-1.69154900	0.68511300	0.09081700
H	-1.83196200	-1.21696400	0.06082500
H	-2.27052700	1.59636200	0.02008500
O	-2.42354600	-0.45305800	-0.04035300
3-im8			
C	0.06059700	0.58295100	0.00000000
H	-0.84836400	1.23108500	0.00000000
O	0.06059700	-0.59109900	0.00000000
3-ts2			
C	2.85221900	-0.90853000	0.42177700
H	2.75746300	-0.40997400	1.38742000

H	3.26690200	-0.20893000	-0.30734800
C	1.46930200	-1.37010100	-0.06776900
C	0.89273900	-2.45625900	0.82697700
H	0.85417700	-2.12055400	1.86314400
H	-0.11482300	-2.73838600	0.51263100
H	1.53287000	-3.33648800	0.76648000
O	3.72356200	-2.01058500	0.59852300
H	3.86238200	-2.41746200	-0.26556200
O	1.66282000	-1.83117800	-1.39662600
H	1.08779400	-2.58772400	-1.56603300
O	0.04214200	0.16750700	1.10689500
H	-0.40976900	1.02779100	1.08999000
O	-1.82928300	0.38633600	-0.98854900
S	-2.98409800	0.00680700	0.20078800
O	-2.66368900	-1.35740000	0.60751100
O	-4.22534800	0.16372200	-0.54543100
O	-2.74622200	1.03427200	1.20993700
C	-0.80410700	-0.45776000	-1.26472000
H	-0.96245500	-1.48977700	-0.94244000
H	-0.46504700	-0.35454900	-2.28717600
C	0.55096800	-0.12983800	-0.11266500
O	0.82597400	0.85321500	-0.90965000
O	2.18501500	1.87666400	-0.21597400
N	1.64536000	3.03254700	-0.09401000
O	2.40650500	3.87172700	0.32995700
3-ts3			
O	-0.98008000	0.93575800	0.80746000
S	-1.51779000	-0.46509100	-0.06051900
O	-1.71954400	0.05186400	-1.40751200
O	-2.72030800	-0.75872600	0.69680600
O	-0.42555900	-1.41165600	0.09105300
C	-0.05933300	1.73907200	0.27827200
H	-0.22842500	2.11437700	-0.90769500
H	0.11754200	2.63595700	0.87459900
O	0.85944900	1.29621300	-0.52856300
O	2.16120000	0.39244400	0.46188900
N	2.68177200	-0.42535400	-0.36246700
O	3.57223100	-1.10162700	0.11249600
3-ts4			
O	0.38908500	-0.94410600	-0.53307400
S	-0.73126800	-0.04298000	0.03337900
O	-0.85825000	-0.22339300	1.46886900
O	-1.93013400	-0.20319600	-0.75973200
O	-0.17980100	1.41441700	-0.25033400

C	1.89199100	-0.66155700	0.08032500
H	0.82148300	1.37436200	-0.11492300
H	2.43342100	-1.46467300	-0.42937200
O	2.21578000	0.54969600	0.01530700
3-ts5			
C	-0.76245200	0.49002200	0.00001000
H	-1.15754900	1.51991200	0.00010300
O	-1.45658000	-0.48180600	-0.00000900
O	1.90875600	-0.00611600	-0.00002300
H	1.73566900	-0.96481200	0.00015900
H	0.37918300	0.40814600	-0.00006800
HCHO			
C	-0.52559800	-0.00001200	0.00000800
H	-1.10704800	-0.93961400	-0.00001600
O	0.67100300	0.00002500	-0.00000200
H	-1.10738600	0.93948300	-0.00001600
P1			
C	1.07352600	0.78339200	-0.58560700
H	0.88412500	1.78347500	-0.19816900
H	0.83038100	0.76008500	-1.65353300
C	0.18980600	-0.23150500	0.14910400
C	0.39531400	-0.19177600	1.66201300
H	0.15200800	0.79411000	2.06003900
H	-0.24228900	-0.93717200	2.14400800
H	1.43777600	-0.42134100	1.88482300
O	2.44708600	0.50844400	-0.37988500
H	2.62766700	-0.37518700	-0.72306700
O	0.53239200	-1.49686600	-0.38280700
H	0.05151400	-2.18280600	0.09791000
O	-1.61134500	1.32185500	0.11066400
H	-2.55424200	1.45574400	-0.08224000
C	-1.27526000	0.06041200	-0.16178500
O	-2.05404000	-0.75843900	-0.58698700

