

Electronic Supplementary Information

Laura M. Castro-Gonzalez¹, Annia Galano^{2*}, Juan Raúl Alvarez-Idaboy^{3*}.

¹ *Centre for Molecular Simulation, Department of Biological Sciences, University of Calgary, Calgary, Alberta T2N1N4, Canada.*

² *Departamento de Química. Universidad Autónoma Metropolitana-Iztapalapa. San Rafael Atlixco 186, Col. Vicentina. Iztapalapa. C. P. 09340. México D. F. México.*

³ *Departamento de Física y Química Teórica, Facultad de Química, Universidad Nacional Autónoma de México, México DF 04510, México.*

Table S1. Main kinetic expressions used for rate constant calculations.

Equation	Description
$k = \sigma \kappa \frac{k_B T}{h} e^{-(\Delta G^\ddagger)/RT}$ <p>σ reaction path degeneracy: 1, κ tunneling corrections¹: computationally determined using an in-house program developed by the authors, k_B, h, T Boltzmann and Plank constants, Temperature: 1.38E-23, 6.63E-34, and 298.15 respectively. ΔG^\ddagger Gibbs free energy of activation: For HAT, it was computationally obtained as the difference of Gibbs free energies (kcal/mol) between the TS and reactants and then energetically corrected by subtracting the factor 4.44, for SET it was determined as shown below, R universal gas constant: 1.986 E-3 kcal/(molK)</p>	<p>Conventional transition state theory (TST)²⁻⁴ was used to compute the rate constants, together with the 1M standard state.</p>
$\Delta G_{ET}^\ddagger = \frac{\lambda}{4} \left(1 + \frac{\Delta G_{reacc}^0}{\lambda} \right)^2$ <p>ΔG_{ET}^\ddagger activation barrier ΔG_{reacc}^0 free energy of reaction λ reorganization therm $\lambda = \Delta E_{elect} - \Delta G_{reacc}^0$, ΔE_{elect} electronic energy of reaction $\Delta E_{elect} = E_{elect\ products} - E_{elect\ reactants}$, $\Delta G_{reacc} = G_{reacc\ products} - G_{reacc\ reactants}$</p>	<p>Marcus theory⁵ was used to calculate the Gibbs free energies of activation for SET reactions.</p>
$k_{app} = \frac{k_D k_{act}}{k_D + k_{act}}$ <p>k_{app} apparent rate constant k_{act} thermal rate constant (obtained from TST)</p>	<p>For high-rate constants (closed to diffusion-limit), the Collins-Kimball theory was used to include the diffusion control⁸ in</p>

k_D steady-state Smoluchowski rate constant ⁶

$$k_D = 4\pi R D_{AB} N_A$$

R reaction distance (i) for SET reactions, it is assumed to be the sum of the radius of the reactants; (ii) for HT reactions, taken from the transition as the distance between the two atoms that are involved in the H transfer. All in Angstroms.

N_A Avogadro number: **6.02E+23**

D_{AB} mutual diffusion coefficient of reactants A and B: free radical and antioxidant, respectively.

It's been calculated from D_A and D_B ⁷ which could be obtained as follows(Stokes-Einstein):

$$D = \frac{k_B T}{6\pi\eta a} \pi r^2$$

k_B Boltzmann constant

T temperature: 298.15

η viscosity of the solvent (water: 8.91×10^{-4} Pa s, pentyl ethanoate: 8.62×10^{-4} Pa s)

a solute radius, calculated via "volume" calculation in Gaussian 09 program In Angstroms

combination with the Smoluchowski ⁶ steady state for irreversible bimolecular reactions, and the Stokes-Einstein approach ⁹ (Stokes-Einstein).

Table S2. Endergonic values of Gibbs Free Energies of reaction (ΔG_R) for RAF and SET mechanism at 298.15 K, in kcal/mol.

Label	Mechanism	Pentyl ethanoate		Water	
		ΔG_R (\bullet OOH)	ΔG_R (\bullet OOCH ₃)	ΔG_R (\bullet OOH)	ΔG_R (\bullet OOCH ₃)
dS-9S1N	RAF	21.55	25.67	18.08	20.73
dS-9S2N	RAF	13.88	16.63	11.74	13.82
dS-9S3N	RAF	12.72	16.10	11.60	13.95
dS-9S4N	RAF	18.43	20.76	17.20	19.05
dS-9S5N	RAF	12.18	14.87	10.23	12.22
dS-9S6N	RAF	10.71	13.88	9.50	11.40
dS-9S1A	RAF	-	-	9.91	13.38
dS-9S2A	RAF	-	-	12.77	12.27
dS-9S3A	RAF	-	-	4.59	7.76
dS-9S4A	RAF	-	-	16.37	18.92
dS-9S5A	RAF	-	-	2.26	4.61
dS-9S6A	RAF	-	-	8.03	11.60
dS-46S1N	RAF	19.30	22.63	16.93	18.28
dS-46S2N	RAF	12.88	16.11	11.79	13.19
dS-46S3N	RAF	12.63	16.49	11.71	13.52
dS-46S4N	RAF	12.56	14.52	11.11	12.90
dS-46S5N	RAF	10.42	12.68	9.55	11.33
dS-46S6N	RAF	9.31	12.41	8.74	10.64
dS-46S1A	RAF	-	-	15.39	17.31
dS-46S2A	RAF	-	-	6.03	9.16
dS-46S3A	RAF	-	-	11.85	14.30
dS-46S4A	RAF	-	-	7.30	11.40
dS-46S5A	RAF	-	-	8.74	11.13
dS-46S6A	RAF	-	-	3.30	6.59
dS-48S1N	RAF	14.45	17.56	12.69	15.57
dS-48S2N	RAF	11.63	14.35	10.33	12.53
dS-48S3N	RAF	17.53	20.91	14.23	16.26
dS-48S4N	RAF	14.11	16.83	13.04	14.72

dS-48S5N	RAF	9.51	11.84	9.23	11.14
dS-48S6N	RAF	7.23	9.77	6.80	8.84
dS-48S1A	RAF	-	-	12.15	17.40
dS-48S2A	RAF	-	-	7.20	9.88
dS-48S3A	RAF	-	-	13.50	16.26
dS-48S4A	RAF	-	-	8.04	10.37
dS-48S5A	RAF	-	-	7.93	10.21
dS-48S6A	RAF	-	-	3.29	7.64
dS-49S1N	RAF	14.30	16.45	14.03	15.71
dS-49S2N	RAF	12.94	15.23	12.02	13.79
dS-49S3N	RAF	13.55	16.67	12.68	13.96
dS-49S4N	RAF	15.27	18.45	14.37	17.03
dS-49S5N	RAF	11.77	15.14	10.87	12.10
dS-49S6N	RAF	10.68	13.07	9.94	11.81
dS-49S1A	RAF	-	-	8.80	11.40
dS-49S2A	RAF	-	-	12.43	14.66
dS-49S3A	RAF	-	-	6.65	9.52
dS-49S4A	RAF	-	-	12.82	15.57
dS-49S5A	RAF	-	-	4.07	7.22
dS-49S6A	RAF	-	-	9.09	6.71
dS-9N	SET	58.37	59.76	10.62	8.40
dS-46N	SET	56.59	57.98	8.43	6.21
dS-48N	SET	51.11	52.50	3.88	1.66
dS-49N	SET	63.93	65.32	15.40	13.18

Table S3. Rate constants ($M^{-1}s^{-1}$) and their diffusion and molar fraction corrections for each derivative.

	Label	Mechanism	k ($\bullet OOH$)	k_{dif} ($\bullet OOH$)	k ($\bullet OOH$)	k ($\bullet OOCH_3$)	k_{dif} ($\bullet OOCH_3$)	k ($\bullet OOCH_3$)
Water	dS-9S1	HAT	1.33E+07	-	1.28E+07	1.12E+07	-	1.08E+07
	dS-9S2	HAT	4.53E+06	-	4.36E+06	6.28E+06	-	6.03E+06
	dS-46S1	HAT	5.59E+06	-	4.49E+06	1.03E+07	-	8.25E+06
	dS-46S2	HAT	8.78E+06	-	7.05E+06	3.04E+06	-	2.44E+06
	dS-46S3	HAT	1.76E+08	-	1.41E+08	3.61E+07	-	2.90E+07
	dS-48S1	HAT	7.02E+06	-	6.04E+06	8.22E+06	-	7.07E+06
	dS-48S2	HAT	2.24E+07	-	1.93E+07	2.58E+07	-	2.22E+07
	dS-48S3	HAT	3.19E+07	-	2.74E+07	-	-	-
	dS-49S1	HAT	2.07E+05	-	1.48E+05	1.89E+05	-	1.35E+05
	dS-49S2	HAT	1.51E+06	-	1.08E+06	8.56E+05	-	6.12E+05
	dS-9A	SET	7.81E+10	7.25E+09	2.83E+08	1.12E+12	7.20E+09	2.81E+08
	dS-46A	SET	1.49E+10	5.14E+09	1.01E+09	3.34E+11	6.95E+09	1.37E+09
	dS-48A	SET	2.89E+09	2.12E+09	2.94E+08	9.53E+10	6.63E+09	9.22E+08
	dS-48N	SET	5.55E+06	5.59E+06	4.81E+06	4.97E+08	4.67E+08	4.01E+08
	dS-49A	SET	4.11E+09	2.71E+09	7.72E+08	1.23E+11	6.76E+09	1.93E+09
Pentyl Ethanoate	dS-9S1	HAT	1.58E+06	-	1.52E+06	3.87E+05	-	3.72E+05
	dS-9S2	HAT	8.26E+05	-	7.94E+05	2.57E+06	-	2.47E+06
	dS-46S1	HAT	7.57E+06	-	6.07E+06	4.86E+05	-	3.90E+05
	dS-46S2	HAT	2.40E+05	-	1.93E+05	4.36E+05	-	3.50E+05
	dS-46S3	HAT	6.62E+06	-	5.31E+06	1.59E+07	-	1.27E+07
	dS-48S1	HAT	1.77E+06	-	1.52E+06	2.00E+06	-	1.72E+06
	dS-48S2	HAT	1.88E+07	-	1.62E+07	2.91E+06	-	2.51E+06
	dS-48S3	HAT	2.82E+07	-	2.42E+07	4.51E+06	-	3.88E+06
	dS-49S1	HAT	5.09E+04	-	3.64E+04	1.10E+04	-	7.87E+03
	dS-49S2	HAT	1.25E+05	-	8.92E+04	1.89E+05	-	1.35E+05

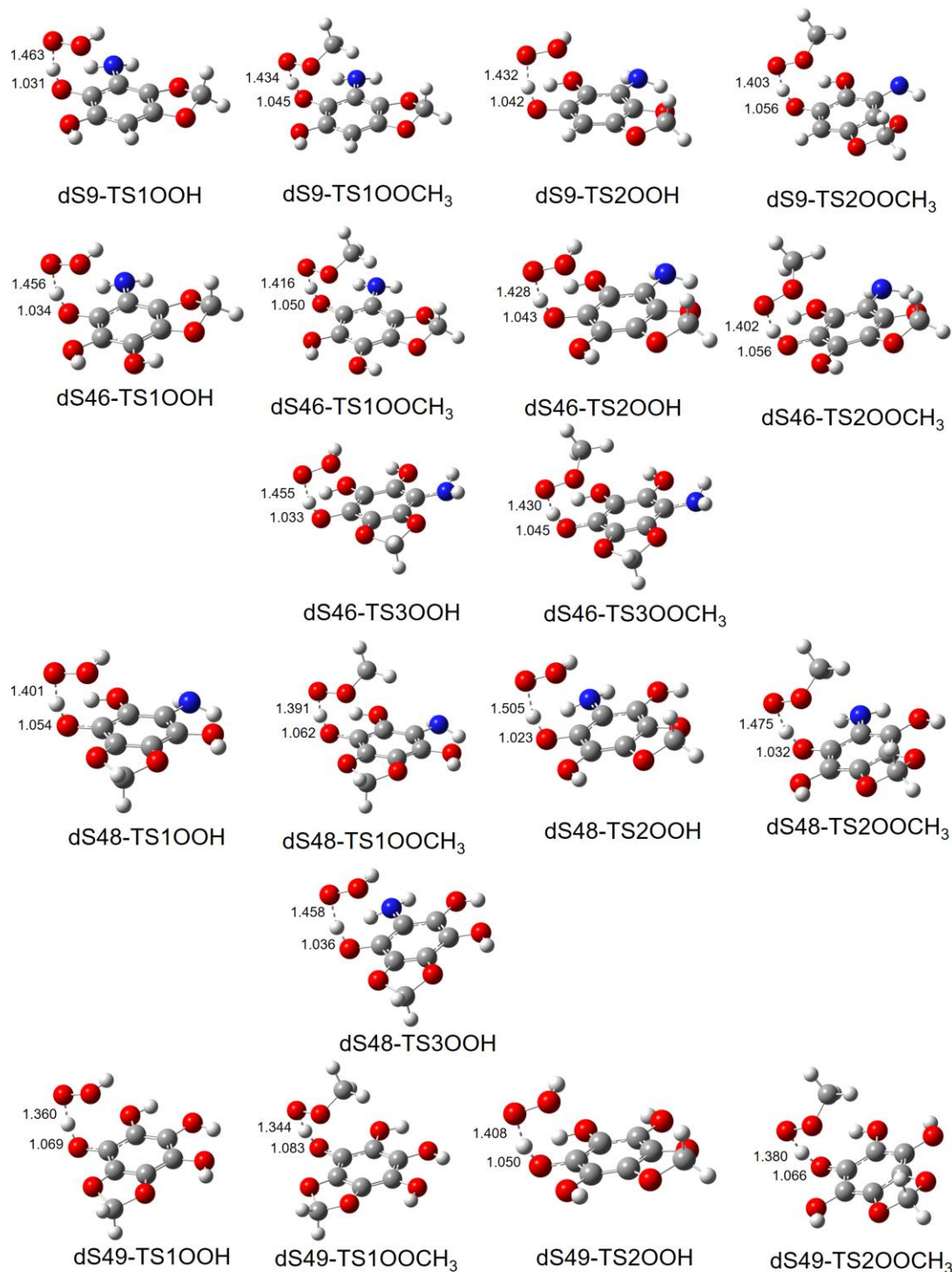


Figure S1. Transition states optimized geometries of each derivative in water solvent.

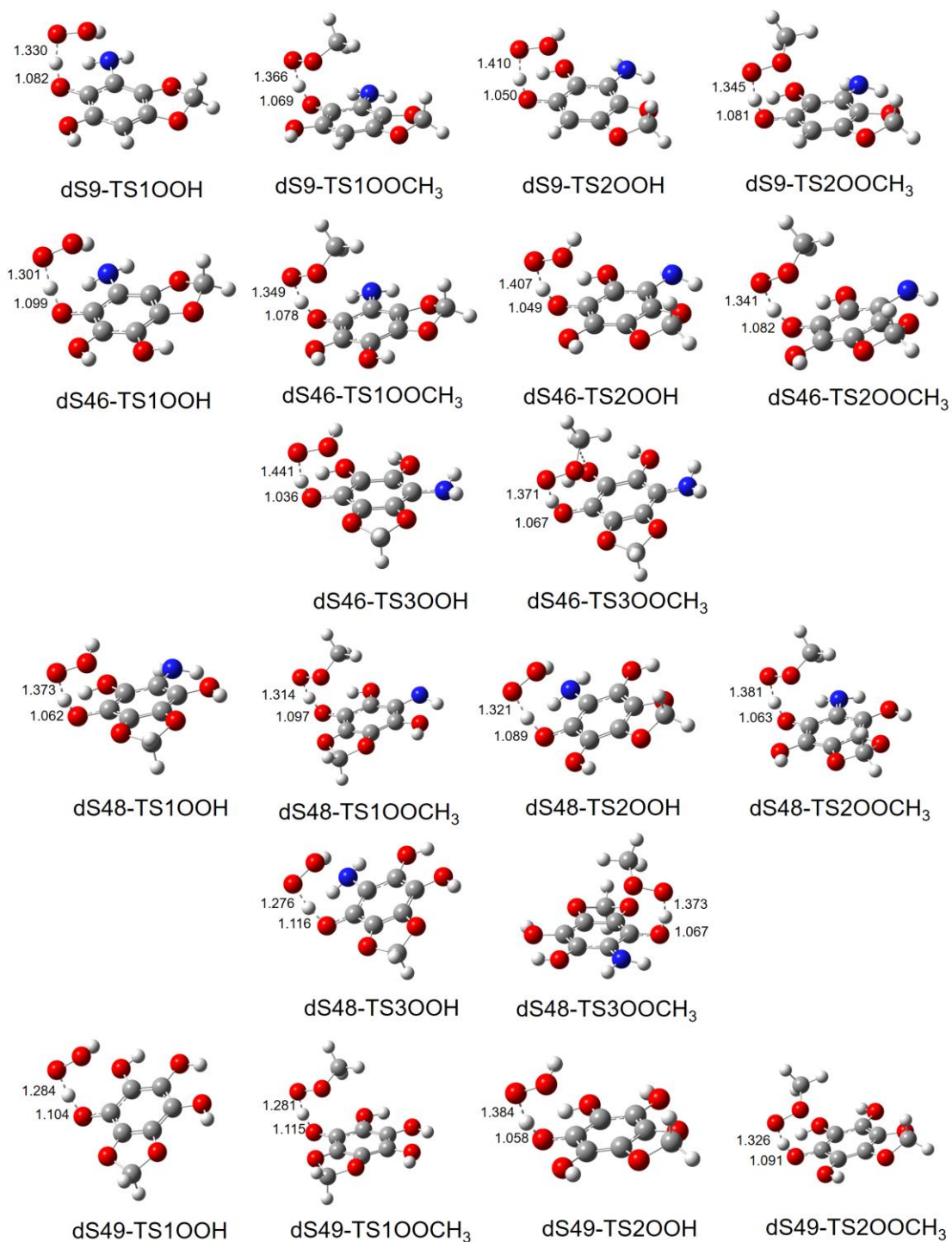


Figure S2. Transition states optimized geometries of each derivative in pentyl ethanoate solvent.

Cartesian coordinates

TS-f-HAT-Water

dS-9S1- OOH

0 2			
C	-0.74307600	-1.30205700	-0.48174900
C	0.50357000	-1.80602400	-0.12298600
C	1.50379400	-0.86407100	0.01826200
C	1.31226100	0.49054700	-0.17071600
C	0.09146500	1.01856500	-0.52976500
C	-0.96048100	0.07665800	-0.68483900
H	0.66780900	-2.86143400	0.03817400
O	-2.17125600	0.52477900	-1.07871000
H	-2.76852200	0.64620700	-0.24690500
O	-1.83200100	-2.09987400	-0.64318900
H	-1.58688000	-3.02159700	-0.50034900
O	2.52129700	1.15772900	-0.03147300
O	2.82238100	-1.08983700	0.31617600
C	3.34929600	0.20926100	0.64531300
H	3.26391000	0.35611500	1.72161800
H	4.36577100	0.28630600	0.28191600
N	-0.14389300	2.35932200	-0.68919200
H	0.66550700	2.92848200	-0.88356100
H	-0.95895700	2.58705300	-1.23804400
O	-3.17002300	0.71398100	1.15873000
O	-2.10519400	0.13883000	1.73180300
H	-1.50399000	0.86146900	1.98368500

dS-9S1- OOCH₃

0 2			
C	-0.60983800	1.40701100	0.49704600
C	0.59792300	1.85236500	-0.03094600
C	1.59801300	0.90271000	-0.09592800
C	1.44346700	-0.40564800	0.32547100
C	0.26156400	-0.87605200	0.85084200
C	-0.79584200	0.07163100	0.92192000
H	0.73225000	2.86866800	-0.37063100
O	-1.97612100	-0.32452400	1.43061300
H	-2.66726100	-0.37741100	0.64799300
O	-1.69633300	2.21174700	0.61080600
H	-1.49538700	3.08799100	0.26141300
O	2.64747600	-1.08235300	0.19253000
O	2.88331300	1.07923400	-0.53364900
C	3.39591100	-0.25592300	-0.70193000
H	3.20915100	-0.57135600	-1.72803400
H	4.44340800	-0.27472600	-0.43040800
N	0.05610100	-2.17617500	1.22734100
H	0.87956700	-2.71538100	1.44533000
H	-0.72987300	-2.33102700	1.83931500
O	-3.19543900	-0.45125300	-0.68282400
O	-2.10687400	-0.06749700	-1.36556100
C	-1.44823300	-1.19945700	-1.96016400
H	-0.49712300	-0.82209100	-2.32624600
H	-1.30895600	-1.96882600	-1.20383000
H	-2.06445300	-1.56527800	-2.77947700

dS-9S2- OOH

0 2			
C	-0.99664700	-0.50924400	-0.79631000
C	0.03485000	-1.46208000	-0.71521300
C	1.24734600	-0.97825600	-0.31316400
C	1.46064300	0.36361600	0.00061000
C	0.47853600	1.32594400	-0.06977000
C	-0.77630500	0.84713700	-0.48431600
H	-0.14423400	-2.49672700	-0.96426600
O	-1.78864500	1.74762400	-0.56828900
H	-2.56735200	1.30466100	-0.93587400
O	-2.23724800	-0.85232100	-1.20634300
H	-2.84179900	-0.98637300	-0.36830600
O	2.77942100	0.56134400	0.32177200
O	2.44399900	-1.64827600	-0.19733800
C	3.29982000	-0.76077800	0.53267200
H	3.24073500	-0.99792100	1.59388800
H	4.30560600	-0.81944200	0.13733800
N	0.67101400	2.65021200	0.29080200
H	1.62997100	2.95799100	0.22106300
H	0.03235100	3.29059200	-0.15767900
O	-3.31019700	-0.98823800	0.98524200
O	-2.20485800	-0.58701500	1.63339900
H	-2.30161400	0.37274900	1.76363300

dS-9S2- OOCH₃

0 2			
C	-0.75093900	-0.42324200	-1.06039400
C	0.23863300	-1.41154400	-0.89653300
C	1.41240900	-0.97728300	-0.35212800
C	1.63507700	0.35278900	0.01178400
C	0.70301900	1.35150400	-0.15320800
C	-0.51680800	0.92137400	-0.70476600
H	0.05263500	-2.43645400	-1.17894900
O	-1.47994100	1.85417800	-0.88918500
H	-2.25285400	1.41696600	-1.27790000
O	-1.96378500	-0.71293600	-1.57051400
H	-2.53388900	-1.13891700	-0.79028900
O	2.91567800	0.49424100	0.48223600
O	2.56387300	-1.69107200	-0.11234600
C	3.35068900	-0.84985700	0.73977600
H	3.13842100	-1.09491000	1.77937600
H	4.39693900	-0.94790600	0.48116700
N	0.89988700	2.66472700	0.24498900
H	1.87102900	2.93943200	0.27712300
H	0.33539400	3.33115100	-0.26157500
O	-2.98620800	-1.45808300	0.49892100
O	-2.05830600	-0.83338700	1.24258200
C	-2.59175600	0.38120800	1.79307600
H	-1.75496200	0.87380900	2.28046800
H	-2.99593400	0.98898800	0.98643300
H	-3.36841600	0.12153200	2.51003600

dS-46S1- OOH

0 2

C	0.67232500	1.18166300	-0.48364200
C	-0.62988700	1.52294900	-0.13615300
C	-1.51740900	0.47250000	-0.00388200
C	-1.15220100	-0.84650400	-0.19523600
C	0.12258000	-1.22478000	-0.55110000
C	1.05048700	-0.15856600	-0.69295300
O	2.31148200	-0.44332700	-1.07621300
H	2.91094200	-0.50733500	-0.23580200
O	1.63931100	2.13077500	-0.60792800
H	1.26545100	2.99724600	-0.40103500
O	-2.27747100	-1.64855600	-0.05760100
O	-2.85213600	0.54497800	0.28939400
C	-3.20689000	-0.81078900	0.63195200
H	-3.08359000	-0.93864600	1.70683500
H	-4.21155500	-1.01515800	0.28609400
N	0.52593200	-2.53164800	-0.70789900
H	-0.21027300	-3.18253400	-0.93620100
H	1.35570200	-2.64428000	-1.27103300
O	3.29355200	-0.58022600	1.16669800
O	2.11715300	-0.29930100	1.74205100
O	-0.93795400	2.84755800	0.04082200
H	-1.77202700	2.93280000	0.51781700
H	1.67828500	-1.15460000	1.89692100

dS-46S2- OOH

0 2

C	-1.06776400	0.02044100	-0.67632000
C	-0.22782200	-1.11778000	-0.61482300
C	1.07269500	-0.88271000	-0.26028200
C	1.53599200	0.39422200	0.02298900
C	0.75711400	1.53629900	-0.03245900
C	-0.57300100	1.30487800	-0.38588800
O	-1.41046100	2.37761600	-0.44805400
H	-2.27449900	2.06867900	-0.75716800
O	-2.35335900	-0.09327400	-1.05732800
H	-2.91636100	-0.43360800	-0.24830800
O	2.87473700	0.33438000	0.30905700
O	2.12326300	-1.77818100	-0.17630900
C	3.12680100	-1.06154200	0.55199600
H	3.00789500	-1.25584000	1.61709500
H	4.10626300	-1.32158200	0.17285000
N	1.22892800	2.80221500	0.31000100
H	2.22166700	2.90815900	0.15572500
H	0.71210000	3.54712600	-0.13577600
O	-3.28354000	-0.73006600	1.09956600
O	-2.07551700	-0.70870100	1.68131000
O	-0.76577000	-2.33292700	-0.89726600
H	-0.11184500	-3.02666900	-0.74564800
H	-1.96663900	0.18461100	2.05213700

dS-46S1- OCH₃

0 2

C	0.50034200	1.27012800	-0.57938200
C	-0.76534500	1.56630300	-0.08720300
C	-1.63654200	0.50049600	0.02451300
C	-1.29055400	-0.79217100	-0.32699500
C	-0.05348300	-1.12549300	-0.82720700
C	0.86491600	-0.04568500	-0.93673700
O	2.08961900	-0.29114500	-1.43067200
H	2.77821200	-0.24732600	-0.63897500
O	1.45039500	2.23374700	-0.70057400
H	1.09137300	3.07764400	-0.39560600
O	-2.40094900	-1.61066700	-0.16933500
O	-2.94021400	0.53330400	0.43715400
C	-3.26004000	-0.85195900	0.68315300
H	-3.03110400	-1.07677600	1.72431100
H	-4.29372700	-1.03319100	0.41977700
N	0.33135600	-2.40652000	-1.14930200
H	-0.42003400	-3.03945200	-1.37805900
H	1.11805000	-2.46014700	-1.77861400
O	3.30325700	-0.23691100	0.67555400
O	2.17027900	-0.03473500	1.36315100
C	1.72838100	-1.25255700	1.98867800
H	0.74720500	-1.02826000	2.39782800
H	1.67762600	-2.03961700	1.23910300
H	2.43338700	-1.50735200	2.77758400
O	-1.05337000	2.86557300	0.24225900
H	-1.89867000	2.91241500	0.70455600

dS-46S2- OCH₃

0 2

C	-0.83999000	-0.09290900	-0.92357300
C	0.02562000	-1.19401600	-0.70790600
C	1.27294900	-0.89130900	-0.23538300
C	1.66660500	0.41803800	0.00960100
C	0.86436200	1.52629000	-0.19999600
C	-0.41288600	1.22589600	-0.67368000
O	-1.27257000	2.25812700	-0.88500600
H	-2.10730000	1.89202100	-1.21307900
O	-2.07592000	-0.27564200	-1.41293300
H	-2.66877200	-0.70792900	-0.65362600
O	2.96674100	0.42424900	0.43788200
O	2.33498300	-1.73995200	0.01515600
C	3.23479400	-0.94447000	0.79484700
H	3.01177300	-1.07870300	1.85236500
H	4.25632000	-1.18948600	0.53527700
N	1.25777500	2.82683700	0.10892700
H	2.25753600	2.96190700	0.05739600
H	0.76974000	3.52492900	-0.43426500
O	-3.11360100	-1.06310500	0.62797200
O	-2.03221100	-0.70889800	1.33969900
C	-2.23913700	0.56837200	1.96930100
H	-1.27455200	0.85010300	2.38231200
H	-2.57849500	1.28152100	1.22094700
H	-2.98205500	0.44777400	2.75561200
O	-0.44878700	-2.43998500	-0.96549900
H	0.20839600	-3.10369600	-0.72287700

dS-46S3- OOH

0 2

C	0.90994000	-0.03607600	-0.68551900
C	0.42883500	-1.35021500	-0.48444400
C	-0.86117400	-1.59689100	-0.05778900
C	-1.76414300	-0.54682500	0.21461200
C	-1.27305800	0.73381800	0.00307100
C	0.00611600	0.98602200	-0.42154000
O	1.23879600	-2.42250100	-0.72381400
O	2.15628600	0.15897800	-1.15694200
O	-1.33051900	-2.87513600	0.12565900
O	0.22279400	2.34048400	-0.46697300
O	-1.91549700	1.93575300	0.26375900
C	-1.10538900	2.89526900	-0.42530200
H	-1.09044300	3.82469700	0.12826200
H	-1.46900700	3.00360600	-1.44677500
H	2.78911400	0.36346200	-0.36604900
H	2.08658600	-2.09934200	-1.05994400
H	-0.63670000	-3.50915000	-0.09424300
N	-3.04962700	-0.80010700	0.60994800
H	-3.21581400	-1.70370900	1.02499700
H	-3.53637400	-0.03603500	1.05279300
O	3.28275400	0.47993800	0.99739600
O	2.13655500	0.36118200	1.67787200
H	2.04391400	-0.58297300	1.89713000

dS-48S1- OOH

0 2

C	0.85107800	-0.38130600	-0.67601700
C	-0.01603300	-1.47138300	-0.44118300
C	-1.32497200	-1.30613400	-0.01702900
C	-1.81333000	0.00027600	0.21566900
C	-0.96978500	1.06464300	-0.01814000
C	0.32380300	0.88826000	-0.44901400
O	0.43232100	-2.74634900	-0.65646800
O	2.09716700	-0.59860600	-1.11866800
O	0.95416800	2.09831800	-0.53189500
O	-1.19760100	2.41054400	0.21368300
C	-0.12590800	3.05249100	-0.48944100
H	0.19321000	3.93150800	0.05471400
H	-0.44126500	3.26291000	-1.51044600
H	2.75964400	-0.52097900	-0.30252100
H	1.33960600	-2.69670400	-0.98868100
O	3.22966200	-0.39968200	1.01152800
O	2.10332800	-0.01317900	1.63510000
O	-3.08976300	0.12091000	0.65655300
H	-3.33462100	1.05083200	0.74480100
N	-2.14026600	-2.40512400	0.24543400
H	-3.12556100	-2.19987500	0.16261300
H	-1.88495900	-3.22411200	-0.28759200
H	1.69244500	-0.82443100	1.98134400

dS-46S3- OOCH₃

0 2

C	-0.69751700	0.03814200	-0.93729700
C	-0.19091400	1.34055000	-0.72212000
C	1.04806800	1.55660500	-0.15652500
C	1.87656300	0.48435700	0.24838900
C	1.36932000	-0.78444100	0.01025500
C	0.13957300	-1.00615000	-0.55418400
O	-0.93319300	2.43149400	-1.07062600
O	-1.90431300	-0.12229400	-1.50674700
O	1.53920400	2.82181700	0.04831400
O	-0.12816100	-2.34950900	-0.57547200
O	1.92721900	-1.99898000	0.38630700
C	1.16064100	-2.95540700	-0.35334400
H	1.03810500	-3.85748200	0.23143000
H	1.63325900	-3.12591300	-1.32010600
H	-2.57383000	-0.44724300	-0.77340000
H	-1.77458900	2.12721600	-1.43939600
H	0.87306500	3.47103000	-0.21003800
N	3.10766800	0.71212100	0.79627500
H	3.25425900	1.62395400	1.20061200
H	3.52067200	-0.05319900	1.30613100
O	-3.13597500	-0.72908700	0.51128300
O	-2.04111900	-0.56327400	1.26314000
C	-2.06197400	0.71618400	1.92192600
H	-1.07630500	0.83145000	2.36431100
H	-2.26477600	1.49187900	1.18673500
H	-2.83539300	0.69309400	2.68759300

dS-48S1- OOCH₃

0 2

C	0.67008200	-0.28198700	-0.92785000
C	-0.13032000	-1.41365400	-0.67616400
C	-1.39135500	-1.32437900	-0.11052600
C	-1.90017200	-0.05044400	0.25434900
C	-1.12287700	1.05450600	0.00550100
C	0.12452300	0.95233700	-0.57226300
O	0.34376800	-2.65950600	-0.99583200
O	1.87851600	-0.42568600	-1.48653400
O	0.69199200	2.18664400	-0.66992600
O	-1.37068500	2.37869900	0.32496900
C	-0.40879100	3.09574100	-0.45826400
H	-0.05957900	3.95895800	0.09258000
H	-0.84230500	3.34259400	-1.42626400
H	2.60779900	-0.21009700	-0.74549600
H	1.22074100	-2.55362400	-1.39057100
O	3.20685900	0.02302600	0.48857700
O	2.10714100	0.25844400	1.22919100
C	1.76063000	-0.89635700	2.01194200
H	0.77438100	-0.68656900	2.41775400
H	1.74894300	-1.77433000	1.36961200
H	2.49473500	-1.00700000	2.80829000
O	-3.12736500	-0.01304700	0.82764200
H	-3.40171700	0.89963100	0.98155500
N	-2.13712100	-2.46002400	0.16839300
H	-3.13217600	-2.29707800	0.21606800
H	-1.90310700	-3.25548500	-0.40732300

dS-48S2- OOH

0 2

C	-0.99721500	-0.39295000	-0.67866400
C	0.05231500	-1.31797800	-0.48625800
C	1.27087100	-0.79490300	-0.15500500
C	1.47278800	0.57686300	-0.01401300
C	0.47659700	1.49756900	-0.19668800
C	-0.79118300	0.99946200	-0.55113600
O	-2.22216600	-0.84132600	-1.03610700
H	-2.84770100	-0.78898400	-0.22797600
O	2.79324300	0.80980900	0.27685500
O	2.47670400	-1.44630200	0.02377900
C	3.29589400	-0.47553300	0.68388500
H	3.17339200	-0.57427800	1.76161100
H	4.32078700	-0.58113000	0.35396100
O	-3.31026100	-0.57677800	1.18785100
O	-2.15201700	-0.23010600	1.76288400
O	-0.21754000	-2.64581300	-0.64245000
H	0.58178200	-3.16510100	-0.49415600
O	0.61774900	2.85531900	-0.07231300
H	1.51620900	3.07547600	0.20010800
N	-1.85225500	1.85832200	-0.68847800
H	-1.62259200	2.82595200	-0.85452300
H	-2.63072500	1.50644700	-1.22503300
H	-2.09145800	0.73975800	1.68863700

dS-48S2- OOCH₃

0 2

C	-0.83517000	-0.16106500	-0.94324300
C	0.07795400	-1.21493000	-0.70626900
C	1.30710300	-0.86238300	-0.22895200
C	1.65209600	0.46859100	0.00094900
C	0.79638300	1.51200000	-0.23014200
C	-0.48287500	1.18890800	-0.72091500
O	-2.06323600	-0.43229200	-1.43544500
H	-2.64169100	-0.80620100	-0.66800400
O	2.95366900	0.52759800	0.43041100
O	2.40295700	-1.66401800	0.03779400
C	3.26043100	-0.82412600	0.81782100
H	3.02328100	-0.94812400	1.87360000
H	4.29422700	-1.03855900	0.58044500
O	-3.10048900	-1.08129300	0.70711800
O	-2.00565600	-0.69727300	1.37059600
C	-2.20903700	0.57953500	1.99888300
H	-1.24883400	0.84649200	2.43135600
H	-2.51791100	1.29979400	1.24351300
H	-2.96992600	0.46708200	2.76881400
O	-0.34160300	-2.48921000	-0.94519300
H	0.34625400	-3.11617000	-0.69183400
O	1.08813000	2.83571300	-0.02004100
H	1.98019600	2.92828200	0.33463000
N	-1.41089600	2.17298900	-0.92041800
H	-1.06344400	3.11369300	-1.01809500
H	-2.19736000	1.92980300	-1.50219900

dS-48S3- OOH

0 2

C	-0.73909500	-0.53862100	-0.67253700
C	-0.97529200	0.86148000	-0.57338800
C	0.04544900	1.71495900	-0.13873000
C	1.31213900	1.23509100	0.17676800
C	1.52702300	-0.13053100	0.04852200
C	0.53578300	-0.98489200	-0.35587400
O	-1.71560200	-1.36235000	-1.09535000
O	-0.25134800	3.05458100	-0.05568200
O	1.00111400	-2.28190800	-0.30700700
O	2.66078600	-0.84878200	0.37524500
C	2.42728200	-2.12190300	-0.24846500
H	2.85617800	-2.90737600	0.35946100
H	2.81965300	-2.09414500	-1.26462800
H	-2.39296600	-1.49045100	-0.32219600
H	0.51218900	3.53409600	0.28870300
O	-3.00156600	-1.39837300	0.99907900
O	-2.03320800	-0.75672100	1.67238800
O	2.24752200	2.12890600	0.59326900
H	3.09005500	1.68964700	0.76327900
N	-2.22545000	1.35219600	-0.84350100
H	-2.29312600	2.34387100	-1.01110700
H	-2.80834900	0.77429600	-1.42999400
H	-2.26679700	0.18837500	1.64768500

dS-49S1- OOH

0 2

C	0.83655600	0.35506800	-0.68210700
C	0.82317600	-1.05861700	-0.53893300
C	-0.30790300	-1.72985000	-0.10910000
C	-1.48813900	-1.03710600	0.20228400
C	-1.47427700	0.33763400	0.05111800
C	-0.35375500	1.00964400	-0.36724100
O	1.97064700	-1.72007000	-0.83824400
O	1.91110800	0.99497900	-1.13900300
O	-0.23235900	-3.09369900	0.00518500
O	-0.59871500	2.35725100	-0.36669400
O	-2.47422000	1.24053100	0.35187800
C	-2.03396100	2.44746900	-0.28901500
H	-2.30970800	3.30090600	0.31597500
H	-2.43605200	2.48192900	-1.30058500
H	2.60006200	1.12625800	-0.33271600
H	1.83881400	-2.66971400	-0.71444100
H	-1.10309200	-3.45403300	0.21634900
O	3.14235400	1.15939000	0.91406200
O	2.12605600	0.67137500	1.65170900
O	-2.54303500	-1.76541600	0.63061700
H	-3.31418700	-1.20490900	0.78630600
H	2.29930800	-0.28061200	1.75100300

dS-49S2- OOH

0 2

C	-1.06401300	-0.00846900	-0.67890300
C	-0.19190000	-1.12118400	-0.60828700
C	1.10131900	-0.85546900	-0.24977400
C	1.54209200	0.43285000	0.02697000
C	0.72079200	1.53916000	-0.03881700
C	-0.60278900	1.29125300	-0.39299300
O	-1.45202100	2.34800900	-0.45662600
H	-2.31326400	2.03304500	-0.76887400
O	-2.34228400	-0.15826000	-1.05759200
H	-2.89223500	-0.53153500	-0.24484600
O	2.87558900	0.40429900	0.31384100
O	2.16911500	-1.72687600	-0.16256000
C	3.16332000	-0.98721800	0.55482200
H	3.06128800	-1.18227200	1.62119400
H	4.14437100	-1.22292900	0.16419400
O	-3.24565500	-0.83699000	1.08354500
O	-2.06462800	-0.65597400	1.69564500
O	1.20427200	2.78578700	0.23977400
H	0.52033500	3.44399300	0.06235500
O	-0.69808800	-2.34904900	-0.88476400
H	-0.03017700	-3.02721700	-0.72322800
H	-2.07364500	0.25380700	2.04099200

dS-49S1- OOCH₃

0 2

C	0.68485200	-0.17271500	-0.94178800
C	-0.00352500	-1.39152000	-0.71165300
C	-1.25740700	-1.40903500	-0.13432200
C	-1.90129500	-0.21854500	0.26197300
C	-1.23449600	0.96536200	0.03130800
C	0.00898300	0.98869200	-0.55435700
O	0.61826800	-2.54343800	-1.08372900
O	1.88839200	-0.15102500	-1.50375100
O	-1.85411300	-2.62911100	0.03531300
O	0.47140700	2.26957500	-0.60418600
O	-1.59610900	2.24737300	0.39891200
C	-0.69968700	3.07449700	-0.35488800
H	-0.42182600	3.94013800	0.23146000
H	-1.15704800	3.32383000	-1.31114700
H	2.60007900	0.15576600	-0.74705800
H	0.04231100	-3.29349200	-0.88364300
H	-2.69284900	-2.53086700	0.50366500
O	3.15424300	0.41860000	0.44829400
O	2.06829100	0.30166100	1.23995400
C	2.05054600	-0.98837300	1.87458700
H	1.08488700	-1.05747300	2.36785700
H	2.16850400	-1.76146400	1.11789600
H	2.86316900	-1.02661700	2.59787900
O	-3.11351300	-0.33500600	0.84616500
H	-3.46998500	0.53096300	1.08215500

dS-49S2- OOCH₃

0 2

C	-0.83366500	-0.11727500	-0.92686600
C	0.06316300	-1.19192000	-0.70272300
C	1.30188100	-0.85822100	-0.22777300
C	1.67198600	0.46038300	0.01405800
C	0.82891700	1.53088200	-0.20505700
C	-0.43962900	1.21455000	-0.68109400
O	-1.30928700	2.23197500	-0.89076100
H	-2.14563800	1.86083000	-1.21012000
O	-2.06111300	-0.33173400	-1.41301200
H	-2.65022000	-0.76818800	-0.63983800
O	2.96526500	0.49721200	0.44272300
O	2.38064400	-1.68222900	0.02591500
C	3.26734100	-0.86657300	0.79927800
H	3.05422700	-1.00333300	1.85819700
H	4.29241400	-1.08731800	0.53247100
O	-3.08438800	-1.11042400	0.62419900
O	-2.01179700	-0.72768900	1.33720700
C	-2.25493800	0.54133500	1.96960300
H	-1.29991400	0.84612900	2.38826800
H	-2.60891300	1.24829600	1.22187800
H	-2.99800100	0.39963100	2.75218900
O	1.23786000	2.80850600	0.04692400
H	0.52761200	3.42331800	-0.17703100
O	-0.37891500	-2.44831100	-0.95499600
H	0.29193900	-3.09677400	-0.70815500

OOH

0 2			
O	0.05481800	0.70576400	0.00000000
O	0.05481800	-0.59543700	0.00000000
H	-0.87708100	-0.88261600	0.00000000
0 1			
O	0.70249100	0.10234900	-0.06934800
O	-0.70259200	-0.10260600	-0.06895400
H	-1.01759100	0.56680300	0.55236500
H	1.01839700	-0.56475100	0.55405000

OOCH₃

0 2			
O	1.17520400	-0.27506700	0.00000500
O	0.16539900	0.53264500	-0.00000200
C	-1.09657500	-0.17967000	-0.00000300
H	-1.85948800	0.59158400	-0.00181000
H	-1.14218700	-0.78848600	-0.89852500
H	-1.14370100	-0.78570000	0.90032800
0 1			
O	1.16978400	-0.22619200	-0.12187200
H	1.40751800	-0.43525200	0.79279800
O	0.02934500	0.60779100	0.02631200
C	-1.12487900	-0.22990600	-0.00183800
H	-1.96686900	0.45298700	0.09303500
H	-1.17750200	-0.76636700	-0.94789700
H	-1.10690700	-0.92471900	0.83757300

TS-f-HAT-Pentyl Ethanoate**dS-9S1- OOH**

0 2			
C	0.46477300	1.68735100	-0.11559800
C	-0.87695700	1.84756500	0.22089000
C	-1.66708000	0.71858700	0.13022400
C	-1.18380300	-0.51696500	-0.26610800
C	0.12898900	-0.69977800	-0.62001400
C	0.98248000	0.43891900	-0.54036800
H	-1.27581400	2.79989000	0.54149200
O	2.24431100	0.33295600	-0.92841800
H	2.81531700	-0.25012200	-0.21827000
O	1.34678500	2.70690000	-0.06303000
H	0.90185200	3.50593000	0.23808900
O	-2.21201700	-1.43079900	-0.29932800
O	-2.99964900	0.61694200	0.37222400
C	-3.25636300	-0.79581600	0.43960400
H	-3.20858200	-1.11014700	1.48318300
H	-4.21343900	-1.01020600	-0.02041600
N	0.68325000	-1.93775300	-0.92253100
H	0.01594200	-2.64852600	-1.18622000
H	1.45720800	-1.88732900	-1.57274500
O	3.23357000	-0.99712800	0.79926100
O	2.08525000	-1.23707500	1.47079500
H	1.58652900	-1.84875500	0.88878800

dS-9S1- OOCH₃

0 2			
C	0.53738100	1.48542300	-0.39072600
C	-0.68969300	1.85086000	0.15742800
C	-1.65824300	0.86526500	0.17016500
C	-1.45220100	-0.41260500	-0.31900300
C	-0.25168000	-0.80245100	-0.86700000
C	0.77638600	0.18319300	-0.89241900
H	-0.87115100	2.84239900	0.54750000
O	1.94299400	-0.14168300	-1.43839600
H	2.67833600	-0.19261200	-0.66374300
O	1.57978600	2.33834900	-0.46698000
H	1.35071900	3.17125500	-0.04230200
O	-2.62382000	-1.13602900	-0.23717200
O	-2.94466000	0.97319800	0.60054800
C	-3.41862600	-0.38139300	0.67471800
H	-3.26018700	-0.75059600	1.68985500
H	-4.45869900	-0.41509400	0.37259200
N	0.01298500	-2.06958300	-1.31679900
H	-0.77633200	-2.63890000	-1.57630500
H	0.81450900	-2.14905200	-1.92356200
O	3.24356100	-0.39889700	0.56243600
O	2.17145900	-0.18201600	1.34487500
C	1.64583500	-1.43009000	1.81495900
H	0.73705400	-1.18100100	2.35790200
H	1.42902000	-2.07896200	0.96723600
H	2.37631000	-1.89296100	2.47720100

dS-9S2- OOH

0 2			
C	-0.98525700	-0.55686400	-0.78396800
C	0.06378800	-1.48965200	-0.69016300
C	1.26849600	-0.97963100	-0.29415000
C	1.45816800	0.37131900	0.00402900
C	0.46059900	1.31708500	-0.08756300
C	-0.78286000	0.80816200	-0.49453900
H	-0.09671800	-2.53010100	-0.92670900
O	-1.81768300	1.67796900	-0.58742800
H	-2.54934100	1.22052900	-1.02659100
O	-2.21753800	-0.90620500	-1.18053900

dS-9S2- OOCH₃

0 2			
C	-0.76270800	-0.40550300	-1.06296300
C	0.22293900	-1.40285100	-0.91119200
C	1.40182800	-0.98262500	-0.36713100
C	1.63602900	0.34402900	0.00960900
C	0.70936400	1.35220900	-0.14276100
C	-0.51079200	0.93428900	-0.69530500
H	0.02898100	-2.42407500	-1.20119200
O	-1.47500100	1.86391600	-0.87268200
H	-2.20168600	1.42998900	-1.34557300
O	-1.96848200	-0.65386600	-1.57790100

H	-2.82058600	-1.04210000	-0.33204200	H	-2.58093500	-1.06669100	-0.78896500
O	2.76562000	0.59738700	0.31864900	O	2.91112500	0.47276400	0.47492100
O	2.46912700	-1.62134000	-0.17354700	O	2.54269200	-1.70172200	-0.13969000
C	3.31117400	-0.711125700	0.53598000	C	3.33819200	-0.87581300	0.71099400
H	3.27272400	-0.93869200	1.60219900	H	3.13896200	-1.13089600	1.75309400
H	4.31643700	-0.75483700	0.13412300	H	4.38375200	-0.97724400	0.44604700
N	0.63062000	2.65131900	0.24170400	N	0.91258900	2.66074700	0.26540500
H	1.57944200	2.98649700	0.17578300	H	1.87787400	2.95030200	0.30360800
H	-0.03103800	3.27602100	-0.19361900	H	0.32638400	3.33559200	-0.20203400
O	-3.32679700	-0.88373600	0.97385400	O	-3.09864800	-1.31347700	0.42741600
O	-2.19984900	-0.57841200	1.64311500	O	-2.08147900	-0.90923400	1.21067400
H	-2.23295200	0.38316100	1.78433800	C	-2.44291900	0.28524100	1.91428300
				H	-1.55612700	0.57951600	2.47002500
				H	-2.73079700	1.05791400	1.20348300
				H	-3.26778400	0.05946500	2.58856400

dS-46S1- OOH

0 2

C	0.23152000	1.55940600	-0.23238100
C	-1.12142900	1.42053100	0.06251500
C	-1.63982000	0.14250100	0.03149300
C	-0.87290000	-0.96671400	-0.28105400
C	0.45469100	-0.86924100	-0.60726100
C	1.02693600	0.43937000	-0.57031700
O	2.29040200	0.60889300	-0.91056800
H	2.95914600	0.14570500	-0.17230400
O	0.81349000	2.77460000	-0.20632500
H	0.15351000	3.42845300	0.05457800
O	-1.67939900	-2.08227500	-0.27805700
O	-2.92723100	-0.23141700	0.25608100
C	-2.85262200	-1.66275800	0.41745900
H	-2.74892400	-1.88502100	1.48037900
H	-3.72730800	-2.11953400	-0.02869900
N	1.28398000	-1.96822500	-0.83561200
H	0.79073000	-2.81930900	-1.06672400
H	2.02142600	-1.78047700	-1.50378200
O	3.50336500	-0.45745600	0.84370000
O	2.43197600	-0.94380400	1.51414600
O	-1.82834300	2.54944800	0.35140200
H	-2.70705700	2.32886300	0.67866200
H	2.07827600	-1.64358500	0.92142700

dS-46S1-OOCH₃

0 2

C	0.44285000	1.31529700	-0.54175000
C	-0.83636300	1.55184700	-0.04956900
C	-1.67181200	0.45918800	0.04394300
C	-1.28279200	-0.81757900	-0.32543300
C	-0.03380900	-1.09300700	-0.82891800
C	0.85612800	0.01866200	-0.92543800
O	2.06722200	-0.18559500	-1.42460700
H	2.78564100	-0.09360300	-0.62679100
O	1.33581500	2.31900600	-0.64444000
H	0.94454300	3.12061600	-0.27646600
O	-2.36061400	-1.66906000	-0.18081300
O	-2.97028800	0.44735400	0.45423400
C	-3.24867900	-0.95057500	0.66946900
H	-3.03124700	-1.18756000	1.71269600
H	-4.27535100	-1.15843900	0.39330000
N	0.41010300	-2.35109800	-1.16731200
H	-0.29686600	-3.02504700	-1.41517300
H	1.21547000	-2.35727600	-1.77493100
O	3.33350900	-0.14685600	0.60462800
O	2.22103500	-0.05408000	1.35665100
C	1.88805600	-1.33968600	1.89505700
H	0.93425800	-1.21047400	2.40140700
H	1.80744000	-2.06423400	1.08559300
H	2.66257000	-1.63723100	2.60080700
O	-1.16328800	2.83330000	0.29505700
H	-2.00577500	2.85349800	0.76088800

dS-46S2- OOH

0 2			
C	-1.06484300	0.05614700	-0.66971700
C	-0.24541700	-1.09795700	-0.62202200
C	1.05771000	-0.88635700	-0.26081300
C	1.55279500	0.37677500	0.03211200
C	0.79523900	1.53417400	-0.01514900
C	-0.53882600	1.32870600	-0.37162400
O	-1.35399900	2.40969600	-0.42785900
H	-2.21350900	2.10911600	-0.75546000
O	-2.34705400	-0.00602500	-1.03989700
H	-2.90774500	-0.44125700	-0.26730400
O	2.88399100	0.28218500	0.31256300
O	2.07838300	-1.80584000	-0.18478800
C	3.10155500	-1.11901500	0.54004300
H	2.99015100	-1.32166600	1.60652500
H	4.07351100	-1.40151200	0.15452600
N	1.28333500	2.79043100	0.33278700
H	2.27379700	2.90700800	0.18028800
H	0.75422500	3.55197900	-0.06556200
O	-3.31479600	-0.73193800	1.04790300
O	-2.12075500	-0.74958200	1.66697300
O	-0.78744800	-2.29765700	-0.92231600
H	-0.15088700	-2.99703000	-0.73758700
H	-2.05873500	0.09878000	2.13745900

dS-46S2- OCH₃

0 2			
C	-0.82936800	-0.11532500	-0.92991700
C	0.05134800	-1.20429700	-0.70746800
C	1.28831200	-0.87910000	-0.22293500
C	1.67100400	0.43268000	0.02708200
C	0.85931000	1.53118700	-0.19904500
C	-0.40880200	1.21003500	-0.68322800
O	-1.27806900	2.22258900	-0.91495200
H	-2.07011600	1.83470800	-1.31491700
O	-2.05432700	-0.28788400	-1.41541800
H	-2.66537300	-0.73056700	-0.63966200
O	2.96284100	0.44744100	0.46009200
O	2.34853200	-1.71848800	0.02898400
C	3.24094200	-0.91863200	0.80780700
H	3.02531100	-1.06207200	1.86771400
H	4.26583100	-1.15577400	0.54840600
N	1.23100800	2.83965600	0.09847700
H	2.22272100	3.01323300	0.03210200
H	0.69946400	3.53174100	-0.40854700
O	-3.15588400	-1.00729200	0.57758500
O	-2.08022200	-0.72265200	1.33429600
C	-2.27161100	0.52760100	2.00999000
H	-1.33343200	0.73586200	2.51826400
H	-2.50363500	1.30584100	1.28473100
H	-3.08432900	0.42098200	2.72695100
O	-0.37643400	-2.45655900	-0.97410200
H	0.28818900	-3.09367800	-0.68996400

dS-46S3- OOH

0 2			
C	-0.88730700	0.24084100	-0.67819000
C	-0.16982800	1.43779600	-0.45193400
C	1.14200900	1.44252700	-0.02625700
C	1.83674900	0.23936400	0.22407600
C	1.12202000	-0.92500700	-0.01359000
C	-0.18298900	-0.93715400	-0.44644700
O	-0.76666000	2.64145900	-0.66856100
O	-2.14296500	0.31746900	-1.13586800
O	1.82643400	2.60614300	0.17480000
O	-0.63151100	-2.22029400	-0.52034700
O	1.53734600	-2.21784500	0.22430200
C	0.57030800	-3.00456700	-0.47499000
H	0.38315600	-3.92305000	0.06756500
H	0.91570100	-3.17649800	-1.49633600
H	-2.80332900	0.09155600	-0.36996900
H	-1.64186900	2.47965700	-1.04584600
H	1.25729400	3.34823000	-0.05931100
N	3.14354600	0.25182400	0.62880000
H	3.48923000	1.11246200	1.02138100
H	3.50672900	-0.58885900	1.04689400
O	-3.33350800	0.00343200	0.96666800
O	-2.20379200	-0.21787700	1.65465200
H	-1.98025700	0.63103300	2.07284100

dS-46S3- OCH₃

0 2			
C	0.69124500	0.00286100	-0.93726100
C	0.23087300	-1.31799400	-0.71966600
C	-0.99299700	-1.59237100	-0.15135200
C	-1.86110600	-0.55374400	0.25785800
C	-1.40533600	0.73475100	0.02263600
C	-0.18725600	1.01470800	-0.54960300
O	1.01721600	-2.37092500	-1.07284100
O	1.87928000	0.18136300	-1.51140500
O	-1.42301100	-2.87176900	0.04922400
O	0.00863900	2.35975900	-0.58185900
O	-2.01747800	1.91231100	0.39641200
C	-1.29785100	2.90384600	-0.33943500
H	-1.20900600	3.80737300	0.25143400
H	-1.79084500	3.06978700	-1.29931100
H	2.56395900	0.53206600	-0.77210100
H	1.79901700	-2.01874500	-1.52026700
H	-0.75052900	-3.48230900	-0.27412200
N	-3.08097500	-0.83219900	0.80667700
H	-3.21982100	-1.76226400	1.16675700
H	-3.54413200	-0.09528100	1.31292700
O	3.15719700	0.74711600	0.44528200
O	2.07908300	0.64114700	1.23753800
C	2.11608800	-0.59013000	1.97219900
H	1.14902800	-0.67124500	2.46244500
H	2.28124800	-1.41998300	1.28738500
H	2.91854100	-0.53759000	2.70704900

dS-48S1- OOH

O 2

C	0.83537500	-0.41039200	-0.66589800
C	-0.06310400	-1.47755900	-0.42739200
C	-1.36700700	-1.28191100	0.00057200
C	-1.82006400	0.03753600	0.22316100
C	-0.95102000	1.07763400	-0.01857100
C	0.34070300	0.87616000	-0.44898500
O	0.35315900	-2.75377200	-0.64626300
O	2.06021600	-0.68435800	-1.10900600
O	0.98341900	2.06828500	-0.54471100
O	-1.16213000	2.41949100	0.19961300
C	-0.07266900	3.04059600	-0.49451000
H	0.26276400	3.91078900	0.05636600
H	-0.38265400	3.27339700	-1.51440500
H	2.75348500	-0.54126300	-0.31692400
H	1.24750300	-2.71304200	-1.01054900
O	3.26427500	-0.45773600	0.95526700
O	2.18816300	0.00326200	1.62318200
O	-3.08978700	0.20244500	0.65916000
H	-3.29601800	1.14077300	0.73991400
N	-2.20512800	-2.35789100	0.26924700
H	-3.18895600	-2.14477800	0.20813500
H	-1.96113700	-3.20205300	-0.22620200
H	1.80910600	-0.77190500	2.07073400

dS-48S2- OOH

O 2

C	-0.92937200	-0.55553700	-0.61054000
C	0.19150000	-1.39232800	-0.36660800
C	1.36851000	-0.76248100	-0.07786100
C	1.48316400	0.62375300	-0.02087000
C	0.42494800	1.46488300	-0.24835200
C	-0.79918800	0.85836300	-0.55657400
O	-2.09546700	-1.08796300	-0.93387500
H	-2.81661100	-0.93500400	-0.13235200
O	2.77568900	0.96236400	0.24098600
O	2.60516500	-1.32263600	0.12630300
C	3.38180500	-0.26309800	0.69112100
H	3.31989800	-0.30633500	1.77897800
H	4.39777000	-0.31711100	0.32041800
O	-3.45042800	-0.60347400	0.97808700
O	-2.53110100	0.14372500	1.63166500
O	0.04042900	-2.73337700	-0.44548300
H	0.87458100	-3.16360400	-0.22819400
O	0.48093200	2.82563900	-0.19654600
H	1.36853200	3.11462800	0.04053800
N	-1.94237300	1.63751700	-0.68316500
H	-1.76417400	2.61419500	-0.87033500
H	-2.64331000	1.24709000	-1.29983000
H	-2.47002100	0.96797000	1.10193900

dS-48S1- OOCH₃

O 2

C	0.69062300	-0.08362700	-0.93627100
C	0.13433600	-1.36515200	-0.69974500
C	-1.10821300	-1.55544400	-0.12093100
C	-1.86272200	-0.41985600	0.26063000
C	-1.33363900	0.82712200	0.02067000
C	-0.09734800	1.00784700	-0.55761200
O	0.85257700	-2.46429800	-1.05760400
O	1.88241500	0.00372200	-1.50722000
O	0.19221500	2.33177700	-0.61446900
O	-1.86259100	2.04766500	0.37414100
C	-1.06656300	2.97907000	-0.36884900
H	-0.90518200	3.87222300	0.22215300
H	-1.54830300	3.18171000	-1.32657100
H	2.60109900	0.32904600	-0.74562800
H	1.65522600	-2.15342200	-1.49827300
O	3.17776400	0.54394600	0.41522000
O	2.09466200	0.55578100	1.21823400
C	2.04356500	-0.64520300	2.00065500
H	1.08959100	-0.61681100	2.52135300
H	2.10798900	-1.51364900	1.34718600
H	2.87044900	-0.63881500	2.70967900
O	-3.06750900	-0.62925400	0.83765800
H	-3.50074100	0.21279800	1.01965500
N	-1.59121200	-2.82965700	0.14911500
H	-2.59534500	-2.89467800	0.21615300
H	-1.19280200	-3.55406500	-0.42847100

dS-48S2- OOCH₃

O 2

C	-0.80638900	-0.28077700	-0.94230500
C	0.16179000	-1.27619600	-0.65419000
C	1.36486600	-0.83707400	-0.18241600
C	1.64562700	0.51546100	-0.00053700
C	0.74344800	1.50540900	-0.28124700
C	-0.51002900	1.09517100	-0.76899600
O	-2.00308400	-0.60873700	-1.42397300
H	-2.62185800	-0.90110700	-0.61057400
O	2.93347700	0.65519600	0.43233100
O	2.48995700	-1.57219900	0.11790100
C	3.30109800	-0.66607200	0.86584300
H	3.06995800	-0.76278700	1.92790800
H	4.34619800	-0.84161100	0.64184100
O	-3.15848700	-0.98864200	0.65933500
O	-2.08232500	-0.64400800	1.38562300
C	-2.28327200	0.63672300	1.99492300
H	-1.35179200	0.86827700	2.50615400
H	-2.49979500	1.37603200	1.22454300
H	-3.10556800	0.56511500	2.70553700
O	-0.15893600	-2.57591800	-0.85258200
H	0.55875700	-3.13484600	-0.53609300
O	0.96900600	2.84294100	-0.12363700
H	1.87027200	2.99202500	0.18038800
N	-1.48958600	2.01890800	-1.00946500
H	-1.20127100	2.97532200	-1.13721400
H	-2.25749900	1.70629600	-1.58265700

dS-48S3- OOH

0 2

C	-0.65383000	-0.64793800	-0.59521900
C	-0.93555200	0.75464200	-0.55214300
C	0.03864600	1.67164000	-0.17440300
C	1.32983200	1.25627200	0.15011300
C	1.60177400	-0.10054000	0.08815800
C	0.65088700	-1.02225300	-0.26379300
O	-1.57304600	-1.50960700	-0.97299300
O	-0.30541700	2.99119500	-0.13792600
O	1.18159600	-2.27677800	-0.17569200
O	2.77179700	-0.72974000	0.42200700
C	2.59464400	-2.05439800	-0.11035500
H	3.04643900	-2.77632800	0.55885500
H	3.00898300	-2.08690900	-1.11918100
H	-2.39691000	-1.54866900	-0.22185200
H	0.45446200	3.51337000	0.14379400
O	-3.16443200	-1.42235200	0.78979000
O	-2.56680000	-0.43855100	1.50665800
O	2.22325600	2.20705500	0.50954700
H	3.08039300	1.81484000	0.71276400
N	-2.24359500	1.17405400	-0.77420100
H	-2.33848600	2.16508100	-0.94740400
H	-2.74530700	0.61770500	-1.45469500
H	-2.69844200	0.36821400	0.96185200

dS-49S1- OOH

0 2

C	-0.69637900	-0.59776300	-0.59965100
C	-0.90035900	0.81161600	-0.52624200
C	0.11011700	1.68093900	-0.16053600
C	1.38889000	1.20768300	0.15733300
C	1.59004600	-0.15763500	0.09754000
C	0.58945700	-1.03078700	-0.25355000
O	-2.14717100	1.27937000	-0.79524300
O	-1.62810500	-1.41812100	-1.02180600
O	-0.19375800	3.00999000	-0.11958600
O	1.05634400	-2.30640300	-0.18267800
O	2.72606700	-0.84930500	0.42446800
C	2.48104700	-2.16067800	-0.11012000
H	2.88957600	-2.90631100	0.56091900
H	2.89574500	-2.21732700	-1.11733900
H	-2.47465600	-1.44674400	-0.31387100
H	-2.12020700	2.24497400	-0.82516900
H	0.59093200	3.52239000	0.10783500
O	-3.22560900	-1.37225500	0.72496200
O	-2.59377800	-0.44116700	1.48195600
O	2.32015200	2.12027700	0.50931200
H	3.16191300	1.69593200	0.71388300
H	-2.83335900	0.40776000	1.07400700

dS-48S3- OOCH₃

0 2

C	-0.69149700	-0.08374600	-0.92148900
C	-0.49507100	1.30149600	-0.63386100
C	0.68770200	1.73977400	-0.02302900
C	1.70598100	0.85318600	0.29519500
C	1.51535300	-0.48546000	-0.01821100
C	0.36293100	-0.93744200	-0.60566200
O	-1.81244800	-0.49300500	-1.50726200
O	0.80935400	3.07889700	0.22151600
O	0.42253100	-2.30394600	-0.71716500
O	2.34989300	-1.54127700	0.26378400
C	1.81440500	-2.59044900	-0.55817200
H	1.93769700	-3.54273200	-0.05723500
H	2.30108700	-2.55445300	-1.53496400
H	-2.58337300	-0.50490200	-0.76979400
H	1.67819700	3.25559200	0.59910700
O	-3.24584200	-0.46513700	0.43268800
O	-2.22776500	-0.13217300	1.24446100
O	2.82014400	1.35335100	0.88881200
H	3.48020300	0.66152600	1.00980500
N	-1.48307800	2.18802000	-0.92430900
H	-1.26465800	3.16964000	-0.89776400
H	-2.20813000	1.89357300	-1.55691800
C	-1.73835500	-1.29469900	1.92775400
H	-0.82701300	-0.98081100	2.43130100
H	-2.48701600	-1.61764800	2.65016400
H	-1.54107400	-2.08558800	1.20663700

dS-49S1- OOCH₃

0 2

C	0.66353400	0.12379100	-0.93578200
C	0.35778600	-1.25539200	-0.74209800
C	-0.83099400	-1.65722300	-0.16127700
C	-1.78743200	-0.72605800	0.26984400
C	-1.50014400	0.60835700	0.07819100
C	-0.32485300	1.02013700	-0.50345100
O	1.26837000	-2.16904900	-1.14369800
O	1.78093700	0.50913500	-1.50400000
O	-1.03689400	-3.00033500	-0.02673600
O	-0.27174200	2.37710400	-0.50341700
O	-2.22965400	1.69710300	0.48560800
C	-1.61975900	2.78333200	-0.22706400
H	-1.61275000	3.66903100	0.39595400
H	-2.14443500	2.92926800	-1.17251200
H	2.44074000	0.93510200	-0.71289200
H	0.92084000	-3.05123700	-0.96274000
H	-1.88880800	-3.16369800	0.39393900
O	2.97619200	1.19329300	0.42132300
O	2.06539000	0.65840800	1.26401900
C	2.51098300	-0.63524300	1.69306400
H	1.70301800	-1.04109800	2.29712600
H	2.70383900	-1.25975100	0.82186300
H	3.41697000	-0.51715000	2.28572000
O	-2.90785200	-1.21213300	0.84920300
H	-3.51211400	-0.49888400	1.08656500

dS-49S2- OOH

0 2			
C	-1.06105400	0.04509600	-0.66883900
C	-0.21347200	-1.08831700	-0.62097800
C	1.08391800	-0.85350300	-0.25248100
C	1.56889000	0.41574400	0.04369200
C	0.77196000	1.54342300	-0.00687400
C	-0.55505300	1.32359800	-0.36321900
O	-1.37180900	2.40257800	-0.40724100
H	-2.23289800	2.11436800	-0.74254600
O	-2.33759900	-0.03567200	-1.04081100
H	-2.89680000	-0.49394300	-0.26872600
O	2.89403400	0.33663100	0.32317100
O	2.11386400	-1.76025000	-0.18133800
C	3.13689300	-1.06361400	0.53513900
H	3.04519400	-1.27738600	1.60106000
H	4.10747400	-1.32616000	0.13256100
O	-3.30640800	-0.80440500	1.01677900
O	-2.12125100	-0.79629400	1.65635500
O	1.25641300	2.77675200	0.27767800
H	0.55823300	3.42462900	0.12453300
O	-0.72633300	-2.29722200	-0.92678900
H	-0.07105300	-2.98311800	-0.75574000
H	-2.10993200	0.03011400	2.16778700

OOH

0 2			
O	0.05493600	0.70787500	0.00000000
O	0.05493600	-0.59823100	0.00000000
H	-0.87897900	-0.87715400	0.00000000
0 1			
O	0.70217600	0.11367200	-0.05920600
O	-0.70217000	-0.11366600	-0.05921600
H	-1.02289000	0.62422800	0.47370000
H	1.02283900	-0.62427100	0.47367700

dS-49S2- OOCH₃

0 2			
C	-0.82424600	-0.13126100	-0.93448300
C	0.08636600	-1.19456200	-0.70899000
C	1.31347800	-0.84160600	-0.21760100
C	1.67912200	0.47751700	0.03324000
C	0.82570200	1.54054200	-0.19629800
C	-0.43211200	1.20136900	-0.68251500
O	-1.31086900	2.20719800	-0.90165700
H	-2.10045200	1.82504600	-1.31268200
O	-2.04315900	-0.32907900	-1.41657100
H	-2.64626700	-0.78672900	-0.63167700
O	2.96369500	0.51301500	0.46584500
O	2.38539200	-1.66305300	0.03504800
C	3.26837500	-0.84868900	0.81040900
H	3.06139500	-0.99722300	1.87116400
H	4.29571300	-1.06656700	0.54450500
O	-3.11814900	-1.06993000	0.57461200
O	-2.05043300	-0.74980000	1.32964500
C	-2.28575300	0.48992400	2.01025500
H	-1.35245900	0.73425500	2.51159700
H	-2.55626100	1.25907900	1.28848900
H	-3.08790800	0.34932000	2.73308600
O	1.19974600	2.82112600	0.04433000
H	0.48896300	3.40933600	-0.23649600
O	-0.30884000	-2.45556000	-0.97570300
H	0.37261600	-3.07725800	-0.69647300

OOCH₃

0 2			
O	1.17464000	-0.27664100	0.00000400
O	0.16488700	0.53524500	-0.00000300
C	-1.09339900	-0.17923800	-0.00000400
H	-1.86365700	0.58642800	-0.00077000
H	-1.14574800	-0.79052100	-0.89735600
H	-1.14641200	-0.78931300	0.89813900
0 1			
O	1.15454900	-0.26336900	0.10618800
H	1.56109200	-0.15766900	-0.76328700
O	0.02903200	0.60326000	0.01284000
C	-1.12569900	-0.22369800	-0.01862400
H	-1.96571900	0.46912600	-0.03929000
H	-1.13314100	-0.84579300	-0.91493300
H	-1.17668200	-0.84260400	0.87702900

SET- Water
Anions-Reagent/Product

dS-9A

-1	1			0	2			
C	-1.42502200	-1.00568100	-0.00147000	C	-1.44796500	-1.02535200	-0.00435000	
C	-0.22360200	-1.71391300	-0.03483600	C	-0.26141500	-1.72265900	-0.03765700	
C	0.91332400	-0.93451700	-0.04738400	C	0.87874000	-0.93020000	-0.04688200	
C	0.86176600	0.44312400	-0.02914400	C	0.86987900	0.46448200	-0.02845900	
C	-0.32279500	1.15314800	-0.00500500	C	-0.28235000	1.19775600	-0.00325700	
C	-1.52421100	0.39947600	0.01788000	C	-1.51636000	0.42965100	0.01881900	
H	-0.20053800	-2.79384900	-0.05299800	H	-0.22176600	-2.80091200	-0.04628200	
O	-2.71428600	0.97289300	0.05386900	O	-2.64125800	0.99167700	0.04876600	
O	-2.62850000	-1.69275700	0.02667800	O	-2.62809900	-1.67077800	0.02004800	
H	-3.29802900	-0.98767500	0.04957300	H	-3.32840200	-0.99701700	0.04774800	
O	2.15740600	0.95733200	-0.12485500	O	2.17135800	0.92864300	-0.12060600	
O	2.24906600	-1.33082500	-0.15843500	O	2.15979900	-1.36352600	-0.10476600	
C	2.96793000	-0.16275000	0.24420600	C	2.97168800	-0.20842700	0.19818100	
H	3.08327300	-0.17296400	1.32972700	H	3.19049100	-0.21797000	1.26446800	
H	3.91309300	-0.11672600	-0.28201400	H	3.85788200	-0.22228200	-0.42263200	
N	-0.37601700	2.54919100	0.05715400	N	-0.35386200	2.55498500	0.03961400	
H	0.40091200	3.00258300	-0.40189800	H	0.45861600	3.07615500	-0.24963300	
H	-1.26042300	2.89782400	-0.28600700	H	-1.24747900	2.95750000	-0.19686900	

dS-46A

-1	1			0	2			
C	0.26624000	-1.43404900	-0.02437800	C	0.19685300	-1.48217400	-0.00972200	
C	1.48267400	-0.71472800	0.00643600	C	1.45918100	-0.76912600	0.01311800	
C	1.42115900	0.68863800	0.01691500	C	1.45685600	0.67627900	0.01215500	
C	0.23179900	1.42452800	-0.00861700	C	0.30198200	1.43077200	-0.01538400	
C	-0.91947200	0.66208300	-0.02734900	C	-0.87191600	0.67562100	-0.02122800	
C	-0.90681200	-0.72087200	-0.03951300	C	-0.92694800	-0.72985800	-0.02813200	
O	2.63915400	-1.34617500	0.03667500	O	2.54534000	-1.40155800	0.03103800	
O	0.30749100	-2.81369900	-0.03810200	O	0.20183000	-2.83454100	-0.03085800	
O	2.62540300	1.37655100	0.06147700	O	2.65571200	1.30417100	0.04052200	
O	-2.21529600	-1.18660600	-0.14094800	O	-2.24140400	-1.11933600	-0.11467900	
O	-2.24275000	1.10329400	-0.14072400	O	-2.12121400	1.17346800	-0.06524400	
C	-2.99136000	-0.04728400	0.25245500	C	-3.00486900	0.05457200	0.17066100	
H	-3.94121400	-0.06024500	-0.26668400	H	-3.84557300	0.11935000	-0.50761500	
H	-3.09553900	-0.05187700	1.33886700	H	-3.29094900	0.06281200	1.21963000	
H	1.25195200	-3.03422300	-0.01509600	H	1.12774600	-3.12236800	-0.01246700	
H	3.30446100	0.68329800	0.06542500	H	3.34724800	0.62329900	0.04917600	
N	0.22840500	2.82760900	0.04809000	N	0.29410900	2.81881900	0.04588800	
H	1.06031300	3.22614600	-0.36399700	H	1.14064200	3.23645700	-0.31374900	
H	-0.59618800	3.22683200	-0.37787000	H	-0.52681800	3.23457500	-0.37122200	

dS-48A

-1 1

C	-1.41852400	-0.69338300	0.01509300
C	-0.24774700	-1.49791000	-0.01890100
C	0.92019400	-0.74364100	-0.03608500
C	0.93016300	0.64082800	-0.04388000
C	-0.21802000	1.39330000	-0.01580300
C	-1.43681500	0.69439100	0.01456600
O	-2.62581000	-1.37348200	0.05329700
H	-2.36953100	-2.31048100	0.02059400
O	2.24317000	1.09153200	-0.14487100
O	2.24115200	-1.19697000	-0.14845900
C	3.00339500	-0.06059000	0.24948600
H	3.10416100	-0.05654700	1.33636500
H	3.95531700	-0.05694000	-0.26609900
O	-0.34805500	-2.80656000	-0.03658800
O	-0.25400300	2.77776900	-0.02209400
N	-2.64952000	1.39925400	0.12423200
H	-2.60749500	2.30468400	-0.32146300
H	-3.42940400	0.86794200	-0.23540100
H	0.64607800	3.12029200	-0.00075400

0 2

C	-1.45758100	-0.70573000	0.01272100
C	-0.24785100	-1.49763900	-0.02124500
C	0.95565900	-0.72161700	-0.03221900
C	0.95228200	0.64054700	-0.03130100
C	-0.22728500	1.37360500	-0.00964100
C	-1.47048800	0.66520000	0.01536400
O	-2.64599600	-1.37583200	0.04565400
H	-2.44595800	-2.32371000	0.01855800
O	2.24586100	1.11226200	-0.13312400
O	2.23275600	-1.18678200	-0.11041200
C	3.03897300	-0.03336800	0.21239200
H	3.22245600	-0.03272200	1.28571600
H	3.94183500	-0.04581200	-0.38299600
O	-0.28870900	-2.75069300	-0.04086400
O	-0.28933800	2.70873600	-0.02108400
N	-2.64911800	1.38778800	0.11357000
H	-2.60112200	2.31443000	-0.28382200
H	-3.46366800	0.87864700	-0.19630400
H	0.59143200	3.10713100	-0.03392900

dS-49A

-1 1

C	0.26054800	-1.40971400	-0.01713600
C	1.43818900	-0.66225100	0.00537700
C	1.46514100	0.74260200	0.00557300
C	0.22850100	1.42744500	-0.02127400
C	-0.92837600	0.68802500	-0.03838500
C	-0.91751900	-0.69606500	-0.03502100
O	2.64618200	-1.33594600	0.04650000
H	3.32294100	-0.64079300	0.06956800
O	0.25535500	-2.78638500	-0.02840400
H	1.16700200	-3.10052300	0.00055500
O	2.60314100	1.40053000	0.04202100
O	0.23197600	2.80528800	-0.02630700
O	-2.22676400	-1.16336700	-0.14893600
O	-2.24494900	1.12769400	-0.13591600
C	-3.00022200	-0.02829500	0.24803600
H	-3.94715400	-0.03243700	-0.27617600
H	-3.10938600	-0.03294900	1.33371500
H	1.16950600	3.05371300	-0.00235500

0 2

C	0.32371600	-1.41873800	-0.01717400
C	1.47123700	-0.65669600	0.00438300
C	1.44288900	0.79315100	0.01255100
C	0.16577800	1.47441400	-0.00661000
C	-0.94324600	0.69942600	-0.02590300
C	-0.86972200	-0.70695700	-0.02683400
O	2.67086200	-1.26689900	0.02534000
H	3.35859400	-0.58133600	0.04329200
O	0.30234600	-2.78065800	-0.02374700
H	1.20678800	-3.11832400	-0.01007100
O	2.51796600	1.43964400	0.03363000
O	0.13438300	2.82589900	-0.01834700
O	-2.10701400	-1.22406900	-0.07349800
O	-2.26175400	1.06805000	-0.10801900
C	-3.01061900	-0.11918900	0.16065900
H	-3.84186500	-0.19227500	-0.52829600
H	-3.30822900	-0.13950700	1.20599300
H	1.05019200	3.14324800	-0.00022900

Neutral-Reagent/Product

dS-9N

0 1				1 2			
C	-1.40933800	-1.00255700	-0.00102500	C	-1.39028300	-1.03748500	-0.00165100
C	-0.20278600	-1.70789300	-0.03571500	C	-0.19444800	-1.74520700	-0.00424800
C	0.93284800	-0.93069800	-0.05064600	C	0.92562600	-0.95442600	-0.00209600
C	0.89590600	0.44740000	-0.03312800	C	0.88007600	0.46731300	0.00652400
C	-0.28555300	1.16287300	-0.00799400	C	-0.29315200	1.19355200	0.00397700
C	-1.45405100	0.38620100	0.01597600	C	-1.44278100	0.40307000	0.00536300
H	-0.18236600	-2.78815100	-0.05118000	H	-0.16654800	-2.82391500	-0.01062400
O	-2.65377100	1.06479300	0.05736400	O	-2.61899500	1.02813500	0.00826500
H	-3.37538400	0.42407400	0.04587900	H	-3.35330400	0.39528600	-0.00131400
O	-2.63384700	-1.63092200	0.02861800	O	-2.58960100	-1.60542000	-0.00482300
H	-2.51552000	-2.58633600	-0.00753700	H	-2.53575100	-2.57180400	-0.01050100
O	2.18690700	0.95277200	-0.12453000	O	2.12218100	0.95511000	0.01150400
O	2.25483000	-1.33834300	-0.14244300	O	2.19940500	-1.33879900	-0.00437800
C	2.99735400	-0.17132100	0.23577300	C	3.02512800	-0.16239200	-0.00304900
H	3.13740300	-0.17699300	1.31725100	H	3.62365200	-0.14888700	0.90061500
H	3.92858800	-0.13935000	-0.31478200	H	3.60872400	-0.13664900	-0.91635900
N	-0.33697800	2.54772800	0.05149800	N	-0.34528800	2.56954300	0.07158900
H	0.47983100	3.00300100	-0.32852000	H	0.47662600	3.03192200	-0.29002600
H	-1.19294100	2.93923200	-0.31311900	H	-1.20130000	2.96848200	-0.28638600

dS-46N

0 1				1 2			
C	0.24460600	-1.42482400	-0.02323000	C	0.23675900	-1.41384900	0.01488800
C	1.42843700	-0.68057000	0.00878800	C	1.45764900	-0.68070200	-0.01163500
C	1.41507400	0.70775100	0.01555600	C	1.46168500	0.68790500	-0.00741800
C	0.21984300	1.44260800	-0.01200000	C	0.23659300	1.43255300	0.01733300
C	-0.92797400	0.67973400	-0.03317700	C	-0.95585100	0.67274700	0.03584700
C	-0.92406500	-0.70158100	-0.04357500	C	-0.95214400	-0.68645200	0.03207300
O	2.65761100	-1.29616800	0.04747900	O	2.65330900	-1.32155800	-0.04355600
O	0.34797100	-2.79278300	-0.03962900	O	0.33129500	-2.73600200	0.02558400
O	2.59005000	1.42370200	0.05604500	O	2.59617700	1.42182200	-0.03096700
O	-2.22494000	-1.16600400	-0.14046900	O	-2.23664700	-1.15777400	0.12211200
O	-2.24054600	1.12613500	-0.12544800	O	-2.22586800	1.14348600	0.10938700
C	-3.00620700	-0.02515000	0.24616000	C	-3.03955300	-0.01062600	-0.20803300
H	-3.94311000	-0.02947500	-0.29514300	H	-3.23741900	-0.00726100	-1.27781500
H	-3.13238400	-0.03494700	1.32902100	H	-3.93068100	-0.00058400	0.40411300
H	-0.52794000	-3.19509800	-0.01850300	H	-0.53508600	-3.16854000	0.03244800
H	2.54031100	-2.25320400	0.00435400	H	2.52906400	-2.27976900	-0.02052900
H	3.33546100	0.81109600	0.03059500	H	3.37078800	0.84278800	-0.04720400
N	0.22010600	2.83764100	0.04668100	N	0.24208200	2.75322100	0.02318200
H	1.05541400	3.24454900	-0.34957400	H	1.11745200	3.25929800	0.01108800
H	-0.60795100	3.24672800	-0.36246600	H	-0.62564500	3.27225900	0.03681500

dS-48N

0 1

C	1.41854200	0.69772300	0.01173600
C	0.22127700	1.42094200	-0.01938900
C	-0.94077600	0.68806800	-0.04057300
C	-0.92434900	-0.69386800	-0.04016700
C	0.24508600	-1.41435300	-0.01451900
C	1.45033100	-0.69482200	0.01241700
O	2.62859700	1.35463800	0.05590200
H	2.47527300	2.30627200	0.01097900
O	-2.22498400	-1.16305700	-0.13785400
O	-2.25127400	1.12988500	-0.14156400
C	-3.01083600	-0.02456200	0.24225700
H	-3.13317700	-0.02472400	1.32549800
H	-3.94883200	-0.03644100	-0.29677900
O	0.30677300	2.78938300	-0.03288200
H	-0.57339500	3.18235000	-0.01848800
O	0.31858700	-2.78540300	-0.01876600
N	2.66861900	-1.37374500	0.11960300
H	2.64350600	-2.29080000	-0.30226100
H	3.44659700	-0.83445300	-0.23147300
H	-0.56753800	-3.16434600	-0.03396000

1 2

C	1.43087000	0.71362200	0.00496400
C	0.25710000	1.44111200	-0.00721300
C	-0.91439000	0.69744600	-0.01510200
C	-0.93463900	-0.71383300	-0.00997300
C	0.19951100	-1.45286400	-0.00004300
C	1.42801400	-0.72079300	0.00851300
O	2.64016900	1.29375000	0.01615200
H	2.55646700	2.25796000	0.00113400
O	-2.22617000	-1.13585800	-0.07192100
O	-2.16266700	1.16469900	-0.05755100
C	-3.04351600	0.02699500	0.10329700
H	-3.44229900	0.04696600	1.11298000
H	-3.80271900	0.05794800	-0.66794900
O	0.34031700	2.79579400	-0.01296700
H	-0.53377500	3.20416400	0.00605600
O	0.30050700	-2.80154300	-0.01054200
N	2.58080300	-1.36989800	0.01575100
H	2.59658600	-2.37992500	0.01451700
H	3.45551900	-0.86431000	0.01530400
H	-0.57034000	-3.21835600	-0.00430900

dS-49N

0 1

C	0.24593000	-1.42861300	-0.01964300
C	1.43044000	-0.68344400	0.00638400
C	1.41265200	0.70444700	0.00665800
C	0.20934500	1.41736900	-0.02053500
C	-0.94481300	0.67059900	-0.04295100
C	-0.92705900	-0.71212900	-0.04105000
O	2.60760900	-1.38838000	0.03967900
H	3.35098000	-0.77393000	0.08494700
O	0.24177100	-2.79659500	-0.02932000
H	1.15232700	-3.11678500	-0.00571800
O	2.62570800	1.34589600	0.04755000
H	2.48816100	2.30118400	0.02687400
O	0.28263500	2.78439600	-0.03044800
H	-0.60047500	3.17036900	0.00085400
O	-2.22530300	-1.18242300	-0.13193700
O	-2.25320200	1.11059100	-0.13537500
C	-3.01492200	-0.04583200	0.24282600
H	-3.94883500	-0.05786100	-0.30320500
H	-3.14535400	-0.04523900	1.32493100

1 2

C	0.25078500	-1.46245400	-0.00002400
C	1.42055500	-0.71812600	0.00002000
C	1.39782600	0.72042800	0.00002300
C	0.20815000	1.45586600	-0.00001900
C	-0.93441100	0.70340500	-0.00008400
C	-0.91313100	-0.72092000	0.00002000
O	2.57936000	-1.37073200	-0.00016500
H	3.33474400	-0.76346700	0.00097200
O	0.20767300	-2.81574000	-0.00007700
H	1.10306900	-3.17889800	0.00021500
O	2.58555500	1.30144900	0.00012100
H	2.50911100	2.26901700	0.00002000
O	0.30858600	2.80781900	-0.00010800
H	-0.56033900	3.22850500	0.00022300
O	-2.15735800	-1.17632700	0.00004500
O	-2.20183700	1.12126600	-0.00011000
C	-3.04522700	-0.04178000	0.00013200
H	-3.63503100	-0.05784500	-0.90907100
H	-3.63466000	-0.05770700	0.90958100

OOH

0 2				-1 1			
O	-2.32936300	-0.31824800	0.52875200	O	-0.00271300	-0.04663300	-0.23994500
O	-1.66852400	-0.30799700	-0.59392300	O	0.00991000	1.33740100	0.18267200
H	-0.79941800	0.20712800	-0.40650400	H	-0.04070100	1.82128500	-0.64798000
O	0.42567300	1.01623100	-0.05719700	O	-2.47334900	-0.64501700	0.16973300
H	1.24124900	0.47622500	0.00917100	H	-2.92852300	-0.49611400	-0.66247800
H	0.32765800	1.46208200	0.79053200	H	-1.50411200	-0.42385500	-0.01103100
O	2.67554700	-0.54048300	0.00922600	O	2.49874500	-0.62346400	-0.04612400
H	3.44974400	-0.11520000	-0.37313300	H	2.70092000	-0.66521000	0.89149800
H	2.95410500	-0.82626400	0.88506500	H	1.51167100	-0.41439800	-0.10070300

OOCH₃

0 2				-1 1			
O	-1.28864400	0.14821000	0.02595600	O	-0.05833400	-0.61003600	0.11827500
O	-2.52254900	0.47009900	-0.18531000	O	0.00433100	0.69589300	0.72364300
C	-1.10053800	-1.28630800	0.14080700	H	1.50813500	-0.86818800	-0.03475000
H	-1.42400700	-1.74428700	-0.78930400	O	2.50592700	-0.97909600	-0.09050700
H	-0.03613700	-1.41893300	0.30514400	H	2.80727900	-0.23940700	-0.62410200
H	-1.68343500	-1.63529100	0.98812400	O	-2.61519600	-0.72489700	-0.27703100
O	2.72463800	-0.91578700	-0.13541600	H	-3.01032900	-0.76253000	0.59731200
H	2.27763200	-0.05873100	-0.02920900	H	-1.62022700	-0.71002900	-0.11950900
H	3.66276600	-0.71533000	-0.08104300	C	0.16616000	1.64116900	-0.31736300
O	1.32338600	1.52199000	0.19114700	H	1.08811000	1.44792400	-0.87093000
H	0.39009300	1.31006800	0.06821300	H	-0.68643800	1.61098700	-0.99923400
H	1.52167200	2.18426000	-0.47778000	H	0.22268400	2.61931500	0.16035500

SET- Pentyl Ethanoate
Neutral-Reagent/Product

dS-9N

0 1				1 2			
C	-1.40407800	-1.00451200	-0.00029200	C	1.38372000	-1.03941000	0.00291000
C	-0.19685900	-1.70860300	-0.03274900	C	0.19562800	-1.75055700	0.00307600
C	0.93990200	-0.93057900	-0.04862900	C	-0.92677500	-0.95346900	0.00217600
C	0.89905100	0.44884600	-0.03080800	C	-0.88178200	0.46840800	0.00040100
C	-0.28523700	1.16104500	-0.00577700	C	0.28940400	1.20002200	0.00293500
C	-1.45328400	0.38320100	0.01512700	C	1.43825400	0.40077800	-0.00478900
H	-0.16465100	-2.78906400	-0.04587500	H	0.15495700	-2.82956200	0.00640800
O	-2.64762800	1.04979900	0.05074900	O	2.61346300	1.01499600	-0.01527400
H	-3.35881500	0.39960400	0.04390500	H	3.34371400	0.37802900	-0.01251000
O	-2.63035200	-1.61915300	0.03052500	O	2.59394800	-1.58952900	0.00893900
H	-2.52999400	-2.57389200	-0.02584000	H	2.56426800	-2.55691800	0.01063800
O	2.17926900	0.95497900	-0.12221000	O	-2.12314000	0.95307200	0.00047600
O	2.25114200	-1.33420100	-0.13873500	O	-2.19291400	-1.33921100	0.00256400
C	2.99224500	-0.16635900	0.22680500	C	-3.02307200	-0.16373200	-0.00741000
H	3.15028900	-0.17053500	1.30804600	H	-3.60812500	-0.14939000	-0.92146000
H	3.92005000	-0.13344700	-0.33181700	H	-3.62764700	-0.14766000	0.89358200
N	-0.34572800	2.54294600	0.04865400	N	0.34813100	2.56453300	-0.05666300
H	0.45477500	3.02221800	-0.33236500	H	-0.46876500	3.07512400	0.24058800
H	-1.22144100	2.93485800	-0.26132700	H	1.22155900	2.99178000	0.20995100

dS-46N

0 1				1 2			
C	0.23823100	-1.42227800	-0.02339400	C	-0.22305200	-1.41172100	-0.01293900
C	1.42336400	-0.68358100	0.00725100	C	-1.45006300	-0.69270600	0.01167800
C	1.41646400	0.70401600	0.01403600	C	-1.46551300	0.67557800	0.00406600
C	0.22226400	1.44237300	-0.01072600	C	-0.24641400	1.43297700	-0.01532200
C	-0.93017100	0.68427000	-0.03143600	C	0.95486000	0.68242200	-0.02656900
C	-0.92828300	-0.69770200	-0.04138000	C	0.95869200	-0.67886600	-0.02667700
O	2.64517900	-1.29839300	0.04441900	O	-2.64013200	-1.32768900	0.04760600
O	0.34181900	-2.78511000	-0.03905500	O	-0.30714300	-2.73553100	-0.02573900
O	2.58793600	1.40580800	0.05041600	O	-2.60111900	1.39266100	0.02255400
O	-2.21984500	-1.16271400	-0.13446400	O	2.23406600	-1.14543900	-0.11794800
O	-2.23367400	1.12870200	-0.12488200	O	2.21235500	1.15707400	-0.09233100
C	-3.00060300	-0.01866000	0.23971100	C	3.04550100	0.00358500	0.18731700
H	-3.93521700	-0.02398700	-0.30767700	H	3.28724400	0.00352300	1.24880600
H	-3.14142800	-0.02717700	1.32283100	H	3.91387200	0.02214200	-0.45888800
H	-0.53292500	-3.18678700	-0.02681800	H	0.56175300	-3.16311500	-0.04080600
H	2.52252000	-2.25413800	0.02121200	H	-2.53165500	-2.28700600	0.01509800
H	3.32243100	0.78179400	0.05517200	H	-3.37162100	0.80828500	0.04440100
N	0.23235900	2.83456800	0.04399700	N	-0.27276500	2.75342600	-0.02258400
H	1.09293100	3.24274700	-0.28895600	H	-1.15645100	3.24622500	-0.01338900
H	-0.57373400	3.26860100	-0.37960100	H	0.57792400	3.29974400	-0.03960600

dS-48N

0 1				1 2			
C	1.42110700	0.69566500	0.01093200	C	-1.43062900	-0.71083700	0.00241800
C	0.22333500	1.41714900	-0.01849700	C	-0.25650500	-1.43832700	-0.01385600
C	-0.94098000	0.68999800	-0.03502200	C	0.91484500	-0.69900500	-0.02263000
C	-0.92527400	-0.69104100	-0.03454900	C	0.93788400	0.71221800	-0.02053800
C	0.24215100	-1.41388100	-0.01399300	C	-0.19511700	1.45304600	-0.00529400
C	1.45007900	-0.69771200	0.01398800	C	-1.42747800	0.72450500	0.00755000
O	2.62072100	1.35042900	0.05038800	O	-2.63131300	-1.29375200	0.02078700
H	2.45941600	2.29944600	0.00716800	H	-2.54528700	-2.25827100	0.00763600
O	-2.21793000	-1.15941800	-0.13334100	O	2.22373500	1.12993300	-0.08276400
O	-2.24208900	1.13383300	-0.13591600	O	2.15794500	-1.16898600	-0.05759100
C	-3.00429100	-0.02057300	0.23578600	C	3.03791100	-0.02999100	0.12411200
H	-3.14346700	-0.02111100	1.31889000	H	3.41045300	-0.04609800	1.14535300
H	-3.93851300	-0.03094600	-0.31187800	H	3.82137600	-0.06684600	-0.62333600
O	0.31342700	2.78058600	-0.03439900	O	-0.35217000	-2.78558900	-0.01170800
H	-0.56437700	3.17549800	-0.03608400	H	0.51298000	-3.21260600	-0.02852700
O	0.30422900	-2.77759900	-0.02604900	O	-0.29208400	2.79522900	-0.01053000
N	2.66386900	-1.37628800	0.12072000	N	-2.57887400	1.37467400	0.02366400
H	2.64704800	-2.30475800	-0.27308800	H	-2.60086500	2.38524000	0.02529400
H	3.45436900	-0.84056700	-0.20418200	H	-3.45752300	0.87538000	0.03022200
H	-0.58518700	-3.14382000	-0.06320200	H	0.57661400	3.21613300	-0.01842000

dS-49N

0 1

C	0.25646000	-1.43040600	-0.02156100
C	1.43062700	-0.66759000	0.00425000
C	1.40331200	0.71790900	0.00382300
C	0.19304300	1.41495300	-0.02281700
C	-0.95201000	0.65667900	-0.04212100
C	-0.92723600	-0.72817600	-0.04191700
O	2.60680800	-1.36094600	0.04411000
H	3.34346300	-0.73998400	0.07943000
O	0.29383700	-2.78610100	-0.02890500
H	1.21712200	-3.06429300	-0.01229800
O	2.60564100	1.36412400	0.04810600
H	2.45960300	2.31698500	0.03254400
O	0.25237900	2.77828700	-0.02868800
H	-0.63437900	3.15363200	-0.02692300
O	-2.21498600	-1.19777500	-0.13136600
O	-2.25223900	1.09334900	-0.12803500
C	-3.00833700	-0.07004000	0.23922400
H	-3.94173600	-0.08352600	-0.30984300
H	-3.15075800	-0.07029300	1.32202900

1 2

C	0.26317600	-1.46272500	0.00235700
C	1.42302000	-0.71048100	-0.00381200
C	1.38807600	0.72189000	0.00288300
C	0.19270100	1.45558000	-0.00136700
C	-0.94442400	0.70212200	-0.00304400
C	-0.91340200	-0.72402500	0.00239000
O	2.58329900	-1.36230600	-0.01392800
H	3.34270100	-0.76138900	-0.01088800
O	0.23292700	-2.80196500	0.00426700
H	1.13057600	-3.16003600	0.01298700
O	2.56758200	1.31369900	0.01175500
H	2.48513700	2.28190300	0.01071200
O	0.31191300	2.79910600	-0.00036200
H	-0.54317200	3.24739000	-0.00914700
O	-2.14668700	-1.18457100	0.00524300
O	-2.21256000	1.11178500	-0.00740200
C	-3.04716900	-0.05757000	0.00018200
H	-3.64064700	-0.08640700	-0.90767600
H	-3.63824600	-0.07620300	0.90990800

OOH

0 2

O	0.05490400	0.70764200	0.00000000
O	0.05490400	-0.59799200	0.00000000
H	-0.87845700	-0.87720500	0.00000000

-1 1

O	0.05522000	0.79117900	0.00000000
O	0.05522000	-0.68199800	0.00000000
H	-0.88352700	-0.87344800	0.00000000

OOCH₃

0 2

O	-0.16433400	0.53477700	-0.00001100
O	-1.17497900	-0.27625300	0.00001500
C	1.09312700	-0.17930100	-0.00001500
H	1.14554900	-0.79177200	-0.89645700
H	1.86243800	0.58710100	-0.00256100
H	1.14776200	-0.78771800	0.89907800

-1 1

O	1.22686700	-0.27766800	-0.00000200
O	0.07085300	0.60163100	0.00006500
C	-1.04900100	-0.21564700	-0.00001500
H	-1.07351500	-0.86255700	-0.88817600
H	-1.07575600	-0.86090900	0.88943900
H	-1.93848500	0.42564600	-0.00167200

References

1. Kuppermann, A.; Truhlar, D. G., Exact tunneling calculations. *Journal of the American Chemical Society* **1971**, *93* (8), 1840-1851.
2. Eyring, H., The Activated Complex in Chemical Reactions. *The Journal of Chemical Physics* **1935**, *3* (2), 107-115.
3. Evans, M. G.; Polanyi, M., Some applications of the transition state method to the calculation of reaction velocities, especially in solution. *Transactions of the Faraday Society* **1935**, *31* (0), 875-894.
4. Truhlar, D. G.; Garrett, B. C.; Klippenstein, S. J., Current Status of Transition-State Theory. *The Journal of Physical Chemistry* **1996**, *100* (31), 12771-12800.
5. Marcus, R. A., Electron transfer reactions in chemistry theory and experiment. *Journal of Electroanalytical Chemistry* **1997**, *438* (1), 251-259.
6. Von Smoluchowski, M., Mathematical theory of the kinetics of the coagulation of colloidal solutions. *Z. Phys. Chem* **1917**, *92*, 129-168.
7. Truhlar, D. G., Nearly encounter-controlled reactions: The equivalence of the steady-state and diffusional viewpoints. *Journal of Chemical Education* **1985**, *62* (2), 104.
8. Collins, F. C.; Kimball, G. E., Diffusion-controlled reaction rates. *Journal of Colloid Science* **1949**, *4* (4), 425-437.
9. a) G. G. Stokes, *Mathematical and Physical Papers*, Cambridge University Press, Cambridge, 1903. b) A. Einstein, Motion of suspended particles in stationary liquids required from the molecular kinetic theory of heat, 1905, vol. 17 c) Einstein, A., Über einen die Erzeugung und Verwandlung des Lichtes betreffenden heuristischen Gesichtspunkt. *Annalen der Physik* **1905**, *322* (6), 132-148.