Malaprade reaction mechanism for Ethylene Glycol oxidation by Periodic Acid based on Density Functional Theory (DFT)

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1. Computation methodology description and rationalization.

Four density functional theory (DFT) methods were applied to determine the kinetic and thermodynamic properties of the Malaprade reaction mechanism: B3PW91[1, 2], CAM-B3LYP,[3] BMK[4] and ωB97XD[5]. The B3PW91[1, 2] was chosen as one of the most popular hybrid DFT functionals that can properly reproduce a wide scope of molecular properties.[6, 7] The CAM-B3LYP functional was chosen because of its known ability to reproduce a long-range interaction as it combines the hybrid qualities of B3LYP for charge transfer systems.[3, 8] The BMK functional was chosen for kinetic calculations, as the one that yields good to excellent results while used for studying organic reactions.[9-11] The ωB97XD[5] functional was chosen to describe the dispersion effects in the atomic system with non-covalent, week interactions. The input files containing the appropriate molecular geometries (the location of the atoms in 3D space) were constructed and define in Cartesian coordinates type of notification, using GaussView software. During optimization process at each step of the computations, the "opt=Cartesian" option was never used.

The localization of the first-order saddle points/transition states was performed according to the following strategy:

1. Optimized substrate or intermediate structures were used to perform the redundant scan-type computations, in which selected interatomic distances were increased or decreased, forcing the interaction between atomic reaction sites. The classic Gaussian commend was used for this purposes: opt=modredundant.
2. The scan-type computations result in the energy diagram in a function of interatomic distances. The approximate bell shape of the energy curve indicates the energy maximum point which was then selected for the ultimate transition state optimization.
3. Using standards Gaussian command: opt=(calcfc, ts, noeigen). The molecular geometry taken from point 2 was used and frequency analysis was performed on top of this computations with Gaussian command freq. The one imaginary frequency defines the proper localization of the first-saddle point, the transition state.
4. The additional IRC analysis were performed with the final transition state structure in both directions (Gaussian command: irc=(reverse, maxpoints=500, calcfc) and irc=(forward, maxpoints=500, calcfc). In result of this analysis, the products and substrates structures were confirmed.

In addition, the unrestricted DFT computations were performed using a valence triple-ζ basis set (6-311+G(2d,p))[12] including diffuse and polarization functions on oxygen and carbon atoms, and polarization functions for hydrogen. In addition, the only full-electron type of basis set: DGDZVP[13, 14] was used to describe all electrons in iodine atom. In order to perform a brief comparison on what extent the computer time can be limited during computation also Weigend's effective core potential (ECP) (DEF2-TZVP)[15, 16], was applied for the iodine atom in parallel.

Based on all the methods used in the study, with both effective core potential (ECP) (DEF2-TZVP) and full basis set (DGDZVP) describing the electronic structure for iodine atom, the same mechanistic picture can be drawn and comparable trends along the potential energy surface, from substrates to products are preserved. However, application of the full basis set (DGDZVP) describing all electrons of the iodine atom lowers the average transition state energies by c.a. 10-20% in comparison with the results given by ECP (DEF2-TZVP) for iodine atom. Computed mean standard deviation for all Relative Gibbs free energy (ΔG [kJ/mol]) is to be c.a. 16 kJ/mol. All the methods provide consistent reaction kinetic information, being in good agreement with experimental values. The rate limiting step of the reaction

(TS2_C) has been located computationally between 93-134 kJ/mol (see Fig. SI1/SI2 and Table S1/S2), while experimentalists provides the energy regime for the Malaprade process to be within 97-168 kJ/mol with unknown measurement error.[17, 18]

Figure SI 1: Comparison of method performance for transition state structures.

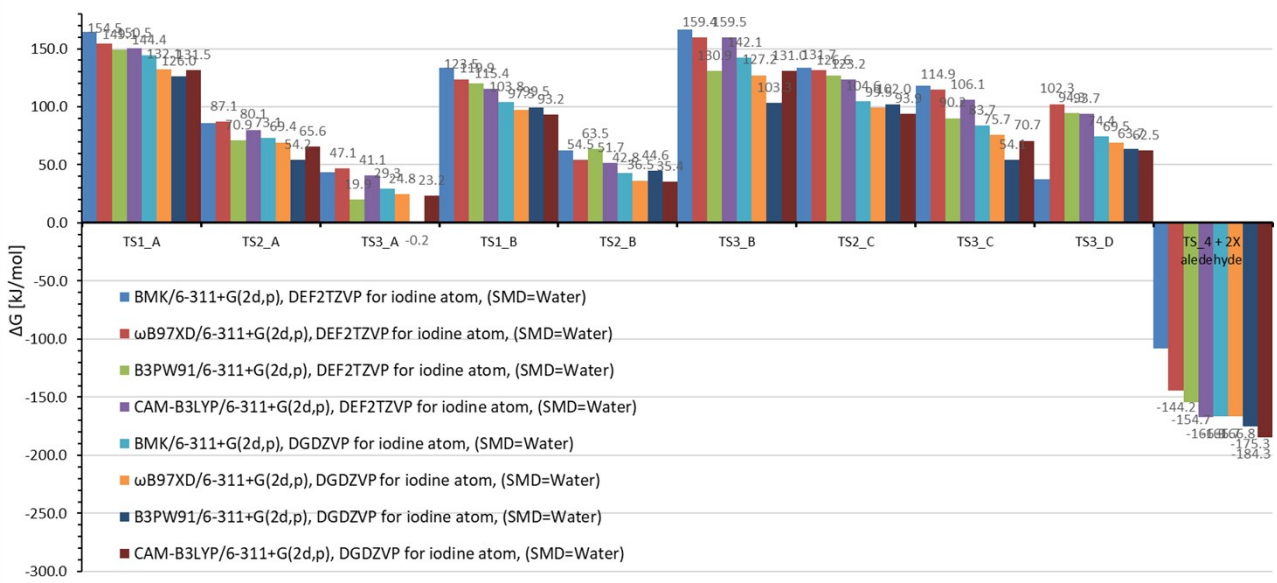

Figure SI 2: Comparison of method performance for intermediate structures.

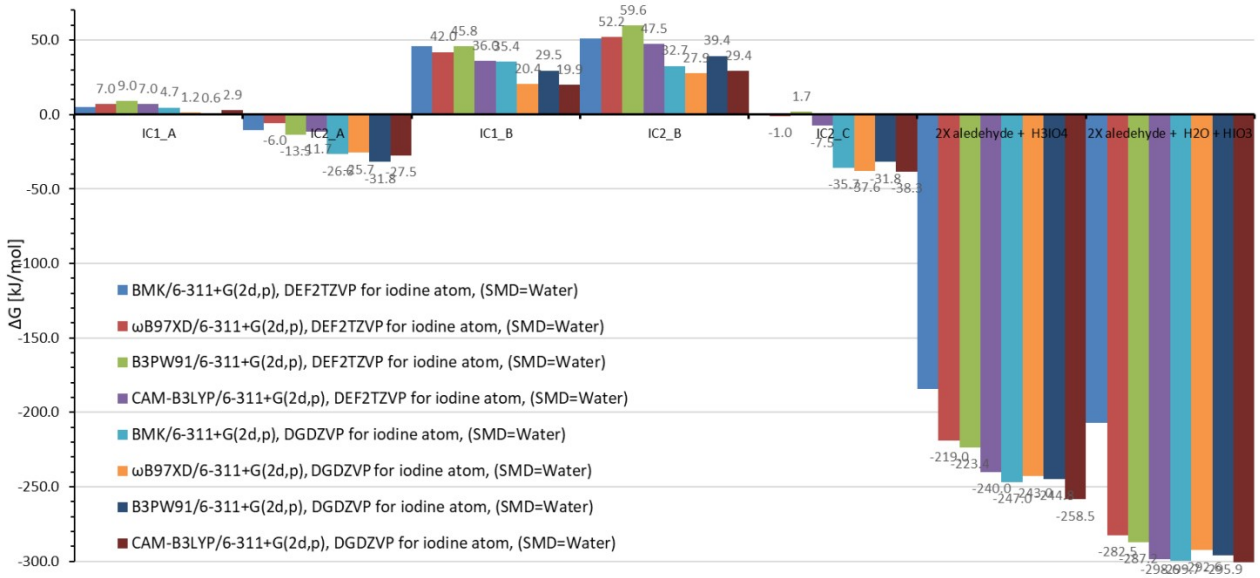

Table S1. Comparison of computed Relative Gibbs free energy (ΔG [kJ/mol]) computed for transition state structures, using different DFT methods.

	ΔG [kJ/mol]										
Method:	**TS1_A**	**TS2_A**	**TS3_A**	**TS1_B**	**TS2_B**	**TS3_B**	**TS2_C**	**TS3_C**	**TS3_D**	**TS_4 + 2X aledehyde**	
BMK/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water)	164.6	86.1	43.3	133.5	62.2	166.6	133.8	118.1	37.3	-108.0	
ωB97XD/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water)	154.5	87.1	47.1	123.5	54.5	159.4	131.7	114.9	102.3	-144.2	
B3PW91/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water)	149.1	70.9	19.9	119.9	63.5	130.9	126.6	90.2	94.3	-154.7	
CAM-B3LYP/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water)	150.5	80.1	41.1	115.4	51.7	159.5	123.2	106.1	93.7	-166.9	
BMK/6-311+G(2d,p), DGDZVP for iodine atom, (SMD=Water)	144.4	73.1	29.3	103.8	42.8	142.1	104.6	83.7	74.4	-166.7	
ωB97XD/6-311+G(2d,p), DGDZVP for iodine atom, (SMD=Water)	132.1	69.4	24.8	97.5	36.5	127.2	99.5	75.7	69.5	-166.8	
B3PW91/6-311+G(2d,p), DGDZVP for iodine atom, (SMD=Water)	126.0	54.2	-0.2	99.5	44.6	103.3	102.0	54.1	63.7	-175.3	
CAM-B3LYP/6-311+G(2d,p), DGDZVP for iodine atom, (SMD=Water)	131.5	65.6	23.2	93.2	35.4	131.0	93.9	70.7	62.5	-184.3	
											Mean SD:
Standard deviation, SD	11.1	10.5	15.4	11.9	10.2	19.7	15.1	20.9	16.4	13.1	14.4

Table S2. Comparison of computed Relative Gibbs free energy (ΔG [kJ/mol]) computed for intermediate structures, using different DFT methods.

	ΔG [kJ/mol]						
Method:	**IC1_A**	**IC2_A**	**IC1_B**	**IC2_B**	**IC2_C**	**2X aledehyde + H3IO4**	**2X aledehyde + H2O + HIO3**
BMK/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water)	5.1	-10.6	45.7	51.3	0.0	-184.5	-207.0
ωB97XD/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water)	7.0	-6.0	42.0	52.2	-1.0	-219.0	-282.5
B3PW91/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water)	9.0	-13.5	45.8	59.6	1.7	-223.4	-287.2
CAM-B3LYP/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water)	7.0	-11.7	36.0	47.5	-7.5	-240.0	-298.6
BMK/6-311+G(2d,p), DGDZVP for iodine atom, (SMD=Water)	4.7	-26.6	35.4	32.7	-35.7	-247.0	-299.7
ωB97XD/6-311+G(2d,p), DGDZVP for iodine atom, (SMD=Water)	1.2	-25.7	20.4	27.9	-37.6	-243.0	-292.6
B3PW91/6-311+G(2d,p), DGDZVP for iodine atom, (SMD=Water)	0.6	-31.8	29.5	39.4	-31.8	-244.8	-295.9
CAM-B3LYP/6-311+G(2d,p), DGDZVP for iodine atom, (SMD=Water)	2.9	-27.5	19.9	29.4	-38.3	-258.5	-303.9

								Mean SD:
Standard deviation, SD	3.2	9.8	10.0	12.2	18.3	13.8	7.5	10.7

2. Kinetic and thermodynamic properties

Table S3. Relative Gibbs free energy (ΔG [kJ/mol]) computed at the B3PW91/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water) (SMD=Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔG [kJ/mol]	0.0	149.1	9.0	70.9	-13.5	19.9
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		119.9	45.8	63.5	59.6	130.9
		TS2_C	**IC2_C**	**TS3_C**		
		126.6	1.7	90.2		
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**2X aldehyde + H2O + HIO3**
		94.3		-223.4	-154.7	-287.2

Table S4. Relative Gibbs free energy (ΔG [kJ/mol]) computed at the CAM-B3LYP/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔG [kJ/mol]	0.0	150.5	7.0	80.1	-11.7	41.1
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		115.4	36.0	51.7	47.5	159.5
		TS2_C	**IC2_C**	**TS3_C**		
		123.2	-7.5	106.1		
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**2X aldehyde + H2O + HIO3**
		93.7		-240.0	-166.9	-298.6

Table S5. Relative Gibbs free energy (ΔG [kJ/mol]) computed at the ωB97XD/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔG [kJ/mol]	0.0	154.5	7.0	87.1	-6.0	47.1
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		123.5	42.0	54.5	52.2	159.4

		TS2_C	**IC2_C**	**TS3_C**		
		131.7	-1.0	114.9		
						2X aldehyde + H2O +
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**HIO3**
		102.3		-219.0	-144.2	-282.5

Table S6. Relative Gibbs free energy (ΔG [kJ/mol]) computed at the BMK/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔG [kJ/mol]	0.0	164.6	5.1	86.1	-10.6	43.3
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		133.5	45.7	62.2	51.3	166.6
		TS2_C	**IC2_C**	**TS3_C**		
		133.8	0.0	118.1		
						2X aldehyde + H2O +
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**HIO3**
		105.2		-232.0	-154.6	-298.2

Table S7. Enthalpy (ΔH [kJ/mol]) computed at the B3PW91/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔH [kJ/mol]	0.0	82.9	-4.7	51.4	-29.7	8.1
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		58.5	-9.6	6.8	3.3	76.0
		TS2_C	**IC2_C**	**TS3_C**		
		58.7	-61.3	35.3		
						2X aldehyde + H2O +
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**HIO3**
		28.4		-174.6	-107.7	-195.4

Table S8. Enthalpy (ΔH [kJ/mol]) computed at the CAM-B3LYP/6-311+G(2d,p), (SMD= Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**

ΔH [kJ/mol]	0.0	86.2	-4.3	61.9	-27.1	30.6
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		55.6	-20.9	-4.6	-7.9	105.4
		TS2_C	**IC2_C**	**TS3_C**		
		56.0	-70.3	50.3		
						2X aldehyde + H2O +
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**HIO3**
		28.5		-190.2	-118.0	-205.1

Table S9. Enthalpy (ΔH [kJ/mol]) computed at the ωB97XD/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔH [kJ/mol]	0.0	87.7	-6.0	66.5	-24.0	34.0
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		60.5	-18.4	-4.4	-7.2	104.3
		TS2_C	**IC2_C**	**TS3_C**		
		62.0	-66.5	56.7		
						2X aldehyde + H2O +
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**HIO3**
		34.7		-171.4	-97.6	-191.4

Table S10. Enthalpy (ΔH [kJ/mol]) computed at the BMK/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔH [kJ/mol]	0.0	96.5	-8.2	65.6	-28.4	30.2
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		70.3	-13.6	0.5	-4.1	110.4
		TS2_C	**IC2_C**	**TS3_C**		
		64.1	-65.4	60.0		
						2X aldehyde + H2O +
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**HIO3**
		37.3		-184.5	-108.0	-207.0

Table S11. Total energy (ΔE [kJ/mol]) computed at the B3PW91/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔE [kJ/mol]	0.0	88.6	-6.1	52.4	-30.3	5.8
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		63.4	-7.1	10.1	5.6	77.4
		TS2_C	**IC2_C**	**TS3_C**		
		64.8	-57.6	36.0		
						2X aldehyde + H2O +
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**HIO3**
		34.0		-180.8	-112.5	-204.6

Table S12. Total energy (ΔE [kJ/mol]) computed at the CAM-B3LYP/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔE [kJ/mol]	0.0	91.5	-6.5	62.5	-27.9	27.9
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		60.0	-18.4	-1.4	-5.6	106.4
		TS2_C	**IC2_C**	**TS3_C**		
		62.0	-66.5	51.4		
						2X aldehyde + H2O +
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**HIO3**
		34.0		-196.7	-123.5	-214.9

Table S 13. Total energy (ΔE [kJ/mol]) computed at the ωB97XD/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔE [kJ/mol]	0.0	93.8	-7.7	67.8	-24.0	32.1
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		65.8	-14.7	-0.5	-3.7	105.8
		TS2_C	**IC2_C**	**TS3_C**		
		68.8	-61.8	58.5		
						2X aldehyde + H2O +
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**HIO3**

		40.9		-177.3	-102.4	-200.5

Table S14. Total energy (ΔE [kJ/mol]) computed at the BMK/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔE [kJ/mol]	0.0	102.9	-10.1	66.8	-28.5	28.2
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		75.6	-10.5	5.1	-1.2	112.1
		TS2_C	**IC2_C**	**TS3_C**		
		70.8	-60.9	61.7		
		TS3_D		**2X aldehyde + H3IO4**	**TS_4 + 2X aldehyde**	**2X aldehyde + H2O + HIO3**
		43.6		-190.4	-112.9	-216.3

Table S15. Relative Gibbs free energy (ΔG [kJ/mol]) computed at the B3PW91/6-311+G(2d,p), DGDZVP for iodine atom, (SMD=Water), (SMD=Water) (SMD=Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔG [kJ/mol]	0.0	126.0	0.6	54.2	-31.8	-0.2
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		99.5	29.5	44.6	39.4	103.3
		TS2_C	**IC2_C**	**TS3_C**		
		102.0	-31.8	54.1		
		TS3_D		**2X aledehyde + H3IO4**	**TS_4 + 2X aledehyde**	**2X aledehyde + H2O + HIO3**
		63.7		-244.8	-175.3	-295.9

Table S16. Relative Gibbs free energy (ΔG [kJ/mol]) computed at the CAM-B3LYP/6-311+G(2d,p), def2-TZVP for iodine atom, (SMD=Water) level of theory.

	Substrates	Substrates		TS1_A	IC1_A	TS2_A
ΔG [kJ/mol]	0.0	**ΔG [kJ/mol]**	0.0	131.5	2.9	65.6
				TS1_B	**IC1_B**	**TS2_B**
				93.2	19.9	35.4
				TS2_C	**IC2_C**	**TS3_C**
				93.9	-38.3	70.7
				TS3_D		**2X aledehyde + H3IO4**
				62.5		-258.5

Table S17. Relative Gibbs free energy (ΔG [kJ/mol]) computed at the ωB97XD/6-311+G(2d,p), DGDZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔG [kJ/mol]	0.0	132.1	1.2	69.4	-25.7	24.8
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		97.5	20.4	36.5	27.9	127.2
		TS2_C	**IC2_C**	**TS3_C**		
		99.5	-37.6	75.7		
		TS3_D		**2X aledehyde + H3IO4**	**TS_4 + 2X aledehyde**	**2X aledehyde + H2O + HIO3**
		69.5		-243.0	-166.8	-292.6

Table S18. Relative Gibbs free energy (ΔG [kJ/mol]) computed at the BMK/6-311+G(2d,p), DGDZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔG [kJ/mol]	0.0	144.4	4.7	73.1	-26.6	29.3
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		103.8	35.4	42.8	32.7	142.1
		TS2_C	**IC2_C**	**TS3_C**		
		104.6	-35.7	83.7		
		TS3_D		**2X aledehyde + H3IO4**	**TS_4 + 2X aledehyde**	**2X aledehyde + H2O + HIO3**
		74.4		-247.0	-166.7	-299.7

Table S19. Enthalpy (ΔH [kJ/mol]) computed at the B3PW91/6-311+G(2d,p), DGDZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔH [kJ/mol]	0.0	58.9	-15.7	33.2	-49.6	-13.2
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		42.9	-29.2	-13.2	-18.5	48.1
		TS2_C	**IC2_C**	**TS3_C**		
		28.4	-95.4	-1.6		
		TS3_D		**2X aledehyde + H3IO4**	**TS_4 + 2X aledehyde**	**2X aledehyde + H2O + HIO3**
		-2.4		-197.0	-128.9	-203.5

Table S20. Enthalpy (ΔH [kJ/mol]) computed at the CAM-B3LYP/6-311+G(2d,p), DGDZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔH [kJ/mol]	0.0	61.7	-14.3	43.2	-47.2	8.4
		TS1_B	IC1_B	TS2_B	IC2_B	TS3_B
		38.1	-40.7	-24.6	-29.0	72.6
		TS2_C	IC2_C	TS3_C		
		24.1	-105.6	11.3		
		TS3_D		2X aledehyde + H3IO4	TS_4 + 2X aledehyde	2X aledehyde + H2O + HIO3
		-3.7		-212.0	-138.2	-212.5

Table S21. Enthalpy (ΔH [kJ/mol]) computed at the ωB97XD/6-311+G(2d,p), DGDZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔH [kJ/mol]	0.0	62.6	-15.2	47.2	-45.0	10.3
		TS1_B	IC1_B	TS2_B	IC2_B	TS3_B
		38.7	-40.8	-24.5	-29.9	69.9
		TS2_C	IC2_C	TS3_C		
		29.1	-103.6	16.0		
		TS3_D		2X aledehyde + H3IO4	TS_4 + 2X aledehyde	2X aledehyde + H2O + HIO3
		1.9		-196.3	-120.5	-201.1

Table S22. Enthalpy (ΔH [kJ/mol]) computed at the BMK/6-311+G(2d,p), DGDZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔH [kJ/mol]	0.0	76.2	-11.4	51.7	-45.2	15.8
		TS1_B	IC1_B	TS2_B	IC2_B	TS3_B
		47.9	-28.9	-17.5	-26.5	85.7
		TS2_C	IC2_C	TS3_C		
		34.2	-100.7	27.6		
		TS3_D		2X aledehyde + H3IO4	TS_4 + 2X aledehyde	2X aledehyde + H2O + HIO3
		7.3		-199.8	-120.7	-207.2

Table S23. Total energy (ΔE [kJ/mol]) computed at the B3PW91/6-311+G(2d,p), DGDZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔE [kJ/mol]	0.0					
		TS1_B	IC1_B	TS2_B	IC2_B	TS3_B
		TS2_C	IC2_C	TS3_C		
		TS3_D		2X aldehyde + H3IO4	TS_4 + 2X aldehyde	2X aldehyde + H2O + HIO3

Table S24. Total energy (ΔE [kJ/mol]) computed at the CAM-B3LYP/6-311+G(2d,p), DGDZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	TS1_A	IC1_A	TS2_A	IC2_A	TS3_A
ΔE [kJ/mol]	0.0	64.8	-16.4	34.5	-50.0	-15.2
		TS1_B	IC1_B	TS2_B	IC2_B	TS3_B

		45.7	-26.1	-9.9	-15.8	49.6
		TS2_C	**IC2_C**	**TS3_C**		
		34.4	-91.7	-0.5		
		TS3_D		**2X aledehyde + H3IO4**	**TS_4 + 2X aledehyde**	**2X aledehyde + H2O + HIO3**
		3.1		-203.0	-133.7	-213.6

Table S 25. Total energy (ΔE [kJ/mol]) computed at the ωB97XD/6-311+G(2d,p), DGDZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔE [kJ/mol]	0.0	69.2	-16.0	48.8	-45.0	8.6
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		42.0	-37.2	-20.4	-26.9	71.8
		TS2_C	**IC2_C**	**TS3_C**		
		35.7	-99.2	18.1		
		TS3_D		**2X aledehyde + H3IO4**	**TS_4 + 2X aledehyde**	**2X aledehyde + H2O + HIO3**
		7.8		-202.2	-125.4	-211.1

Table S26. Total energy (ΔE [kJ/mol]) computed at the BMK/6-311+G(2d,p), DGDZVP for iodine atom, (SMD= Water) level of theory.

	Substrates	**TS1_A**	**IC1_A**	**TS2_A**	**IC2_A**	**TS3_A**
ΔE [kJ/mol]	0.0	82.6	-12.1	53.2	-45.2	13.9
		TS1_B	**IC1_B**	**TS2_B**	**IC2_B**	**TS3_B**
		51.6	-24.0	-13.2	-22.6	87.5

	TS2_C	**IC2_C**	**TS3_C**		
	41.0	-96.5	28.8		
	TS3_D		**2X aledehyde + H3IO4**	**TS_4 + 2X aledehyde**	**2X aledehyde + H2O + HIO3**
	13.3		-205.5	-125.4	-217.4

3. Cartesian coordinates and thermochemistry.

Table S27. Molecular geometries optimized at the B3PW91/6-311+G(2d,p), (SMD=Water) level of theory.

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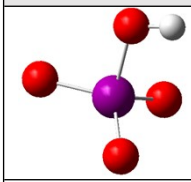
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Cartesian coordinates:
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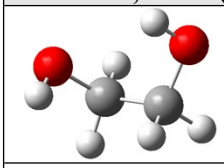
Ethane-1,2-diol (ethylene glycol)

Thermochemistry:
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Cartesian coordinates:
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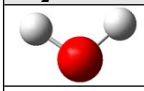
H_2O



Thermochemistry:

Zero-point correction= 0.021141 (Hartree/Particle)
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Thermal correction to Enthalpy= 0.024921
Thermal correction to Gibbs Free Energy= 0.003488
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Sum of electronic and thermal Free Energies= -76.441145

Cartesian coordinates:

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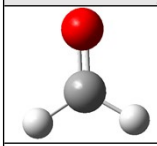
O	0.00000000	0.00000000	0.11792700

Formaldehyde



Thermochemistry:

Zero-point correction= 0.027009 (Hartree/Particle)
Thermal correction to Energy= 0.029874
Thermal correction to Enthalpy= 0.030819
Thermal correction to Gibbs Free Energy= 0.005350
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Cartesian coordinates:

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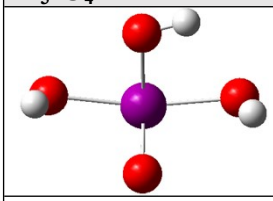
H_3IO_4



Thermochemistry:

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Thermal correction to Gibbs Free Energy=	0.012517
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Cartesian coordinates:

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H	2.31099600	-0.09066100	0.70070700
H	-2.28902900	0.14446100	0.75077300
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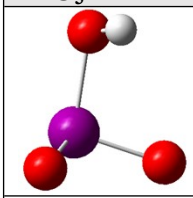
HIO_3



Thermochemistry:

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Cartesian coordinates:

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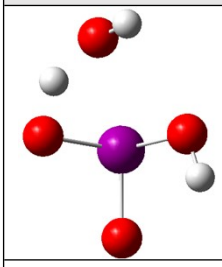
TS4



Thermochemistry:

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Cartesian coordinates:

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H	-1.60836200	-0.80689700	0.64609400
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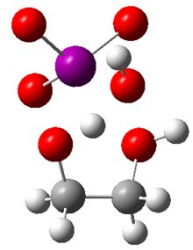
TS1_A



Thermochemistry:

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O -1.37412000 -1.27181800 0.27675000
C -2.57727000 -0.47845400 0.23023200
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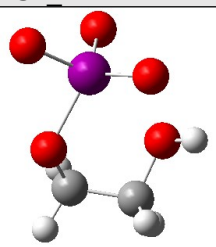
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Thermal correction to Enthalpy= 0.095396
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O 0.70296100 1.28544500 -0.35497600
O 1.66057000 -1.13590000 0.28759300
C 2.60678300 -0.20315300 -0.24462200
C 2.06378200 1.14486600 0.12578500
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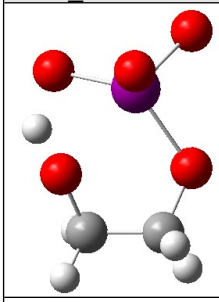
TS2_A



Thermochemistry:

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Cartesian coordinates:

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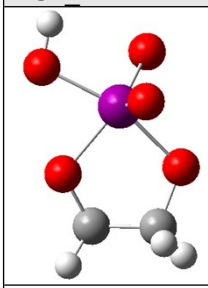
C	-2.40826200	0.44510400	-0.17679000
C	-2.14112900	-1.02750200	0.06845100
H	-2.51048600	0.65317000	-1.24205100
H	-3.30185000	0.75315700	0.36288300
H	-2.24097800	-1.28606400	1.12102100
H	-2.78670900	-1.64571700	-0.55134100
H	-0.55385900	1.75210000	-0.43830600
O	0.57610900	1.57476300	-0.89962000

IC2_A



Thermochemistry:

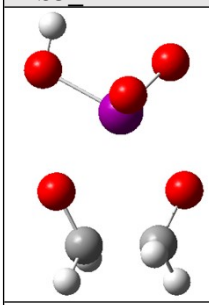
Zero-point correction= 0.085096 (Hartree/Particle)
Thermal correction to Energy= 0.093993
Thermal correction to Enthalpy= 0.094937
Thermal correction to Gibbs Free Energy= 0.050524
Sum of electronic and zero-point Energies= -752.722163
Sum of electronic and thermal Energies= -752.713266
Sum of electronic and thermal Enthalpies= -752.712322
Sum of electronic and thermal Free Energies= -752.756735

Cartesian coordinates:

0 1

I	0.42516900	-0.09232400	0.00359200
O	1.23366500	-0.89004400	-1.34687600
O	1.59387900	1.42073600	0.02055100
O	0.80611400	-0.66884800	1.62290200
O	-0.84159500	1.34862300	-0.01583700
O	-1.15937000	-1.18769500	-0.25166400
C	-2.33754400	-0.51365900	0.18774400
C	-2.20028900	0.93729900	-0.23693100
H	-2.43600700	-0.60979600	1.26937900
H	-3.18263600	-0.97689800	-0.31564200
H	-2.42467000	1.06888700	-1.29358600
H	-2.81935500	1.58250000	0.38191800
H	2.49417300	1.10445300	-0.16993300

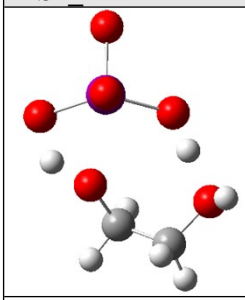
TS3_A



Thermochemistry:

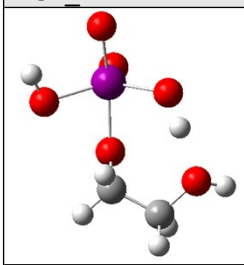
Zero-point correction= 0.081026 (Hartree/Particle)
Thermal correction to Energy= 0.090446
Thermal correction to Enthalpy= 0.091390
Thermal correction to Gibbs Free Energy= 0.045643
Sum of electronic and zero-point Energies= -752.700843

Sum of electronic and thermal Energies= -752.691424 Sum of electronic and thermal Enthalpies= -752.690479 Sum of electronic and thermal Free Energies= -752.736226
Frequency: Infrared:
-713.93 1691.0683
Cartesian coordinates:
0 1 I 0.48315800 -0.06884900 -0.01011100 O 1.54859700 -1.16575900 -0.90799100 O -1.12830900 1.43108200 -0.03568800 O -1.22945400 -1.32532600 -0.29310200 C -2.37284900 -0.80435100 0.08852300 C -2.34283700 0.96784700 -0.19273700 H -2.58066400 -0.88052400 1.15485500 H -3.19410200 -1.01535100 -0.59432800 H -2.73653300 1.06405100 -1.20372800 H -3.01465200 1.20494800 0.63284200 O 1.49163700 1.54005700 -0.26904400 H 2.42100500 1.29821700 -0.43077800 O 0.79149000 -0.35547100 1.70611500

TS1_B

Thermochemistry:
Zero-point correction= 0.105481 (Hartree/Particle) Thermal correction to Energy= 0.115991 Thermal correction to Enthalpy= 0.116935 Thermal correction to Gibbs Free Energy= 0.068496 Sum of electronic and zero-point Energies= -829.112109 Sum of electronic and thermal Energies= -829.101600 Sum of electronic and thermal Enthalpies= -829.100655 Sum of electronic and thermal Free Energies= -829.149094
Frequency: Infrared:
-1486.28 2462.5668
Cartesian coordinates:
0 1 I 0.83869900 -0.05516400 0.03154100 O 0.85870700 -0.36050900 1.76624600 O 1.04319200 1.70316300 -0.49978900 O -2.58750100 -1.29108500 -0.10710900 O -0.98078700 1.15118400 0.37859900 C -2.20082300 1.07166300 -0.36237500

C	-3.11904100	0.02005700	0.18737200
H	-1.99571300	0.89378600	-1.42090100
H	-2.68962100	2.04307000	-0.26729400
H	-3.22754000	0.12896700	1.26530000
H	-4.09597600	0.10933600	-0.28799600
H	-2.67754000	-1.86574700	0.66441600
H	-0.07607700	1.87391900	-0.14154600
O	2.35265100	-0.69766400	-0.60076300
O	-0.25212500	-1.20064400	-0.92379300
H	-1.24248400	-1.24554100	-0.54076600

IC1_B



Thermochemistry:

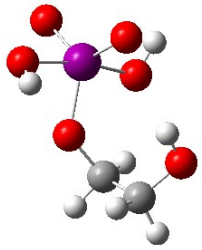
Zero-point correction= 0.110266 (Hartree/Particle)
Thermal correction to Energy= 0.121504
Thermal correction to Enthalpy= 0.122448
Thermal correction to Gibbs Free Energy= 0.072900
Sum of electronic and zero-point Energies= -829.141968
Sum of electronic and thermal Energies= -829.130730
Sum of electronic and thermal Enthalpies= -829.129786
Sum of electronic and thermal Free Energies= -829.179334

Cartesian coordinates:

0 1

I	0.71523000	-0.09939100	-0.00416700
O	0.76433000	-0.94261400	1.54646800
O	1.77566300	1.37278400	0.63378500
O	-2.74882400	-0.94594000	0.31407900
O	-0.61356000	1.25709300	-0.12625300
C	-1.94319400	1.09600200	-0.69400300
C	-2.92774900	0.47593000	0.25464500
H	-1.88360800	0.55938200	-1.63809200
H	-2.23784600	2.12610400	-0.89196400
H	-2.81681800	0.90765700	1.24918800
H	-3.93114900	0.69547900	-0.11638600
H	-2.88674200	-1.25148900	1.21855500
H	1.39277100	1.72282000	1.45615000
O	1.89473200	-0.33129700	-1.29344200
O	-0.44608600	-1.35463200	-0.83296800
H	-1.32819300	-1.36698000	-0.35381900

TS2_B



Thermochemistry:

Zero-point correction= 0.110269 (Hartree/Particle)
Thermal correction to Energy= 0.121226
Thermal correction to Enthalpy= 0.122171
Thermal correction to Gibbs Free Energy= 0.072413
Sum of electronic and zero-point Energies= -829.135496
Sum of electronic and thermal Energies= -829.124539
Sum of electronic and thermal Enthalpies= -829.123595
Sum of electronic and thermal Free Energies= -829.173353

Frequency: Infrared:

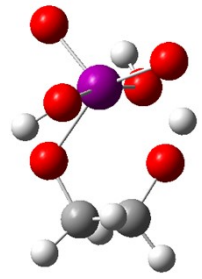
-190.11 201.3241

Cartesian coordinates:

0 1

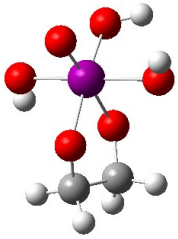
I	0.72482400	-0.05714800	0.01895400
O	0.61467600	-0.81824900	1.60763400
O	1.37419000	1.61494500	0.69654300
O	-2.80624200	-0.70933400	0.88217400
O	-0.71984900	1.01098500	-0.55685300
C	-2.01702100	0.55963300	-1.05885300
C	-3.01663800	0.42624000	0.05455100
H	-1.90494200	-0.35386900	-1.63101800
H	-2.30915200	1.37212400	-1.72426800
H	-3.03456300	1.34065000	0.65258100
H	-3.99766700	0.30088500	-0.40632100
H	-2.02702800	-0.55820100	1.43161500
H	0.74759700	1.98332800	1.34208900
O	2.17042900	-0.16398100	-0.98437100
O	-0.13922900	-1.51482800	-0.88829700
H	0.36022000	-2.32761800	-0.69805400

TS2_C



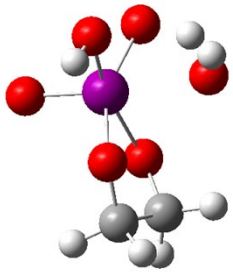
Thermochemistry:

Zero-point correction= 0.107188 (Hartree/Particle) Thermal correction to Energy= 0.117104 Thermal correction to Enthalpy= 0.118048 Thermal correction to Gibbs Free Energy= 0.072425 Sum of electronic and zero-point Energies= -829.111349 Sum of electronic and thermal Energies= -829.101434 Sum of electronic and thermal Enthalpies= -829.100490 Sum of electronic and thermal Free Energies= -829.146113
Frequency: Infrared:
-1652.38 2710.7072
Cartesian coordinates:
0 1 I -0.49124900 -0.01724100 0.03497600 O -0.94448200 1.62516800 -0.65582100 O -0.06891400 0.95032100 1.65009400 O 1.18450800 0.85808700 -0.88302100 O 0.88634900 -1.25618300 0.59920400 C 2.21958600 -0.93873300 0.15943900 C 2.35645100 0.55303800 -0.12718200 H 2.42824500 -1.51690400 -0.73940600 H 2.88802200 -1.22908900 0.96744200 H 2.39366800 1.15447500 0.77830700 H 3.23204200 0.73124500 -0.74658900 H 0.36607400 1.71076800 -0.85939100 H 0.33685800 0.33492200 2.28408500 O -1.91072300 -0.83194000 0.69044000 O -0.61461100 -0.89520000 -1.66808800 H -1.32197200 -1.55950800 -1.59415800

IC2_C

Thermochemistry:
Zero-point correction= 0.110639 (Hartree/Particle) Thermal correction to Energy= 0.121389 Thermal correction to Enthalpy= 0.122333 Thermal correction to Gibbs Free Energy= 0.075041 Sum of electronic and zero-point Energies= -829.160297 Sum of electronic and thermal Energies= -829.149547 Sum of electronic and thermal Enthalpies= -829.148603 Sum of electronic and thermal Free Energies= -829.195895
Cartesian coordinates:
0 1

I	0.40110000	-0.05403300	-0.05416200
O	1.55888800	-0.83223900	-1.13989000
O	-1.11411900	-0.72845500	-1.05476700
O	-0.96757300	0.76148800	1.05917600
C	-2.25810000	0.72737600	0.44268100
C	-2.35489000	-0.55389800	-0.36415400
H	-2.37769100	1.60728900	-0.18915200
H	-2.99252200	0.73152100	1.24547800
H	-2.53062800	-1.41649200	0.27941700
H	-3.13632700	-0.47647900	-1.11688600
O	0.38079300	-1.56691300	1.11650900
H	-0.24516100	-1.39966800	1.84161500
O	0.36837500	1.61959600	-0.99958100
H	0.89579600	1.52244200	-1.81047000
O	1.64670700	0.70079200	1.17366300
H	1.82160500	1.62009200	0.90853200

TS3_D



Thermochemistry:

Zero-point correction= 0.107051 (Hartree/Particle)
Thermal correction to Energy= 0.117163
Thermal correction to Enthalpy= 0.118107
Thermal correction to Gibbs Free Energy= 0.071730
Sum of electronic and zero-point Energies= -829.122032
Sum of electronic and thermal Energies= -829.111920
Sum of electronic and thermal Enthalpies= -829.110976
Sum of electronic and thermal Free Energies= -829.157353

Frequency:	**Infrared:**
-1616.11	2436.7242

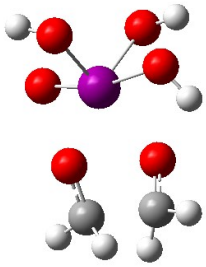
Cartesian coordinates:

0 1

I	-0.37030800	-0.12916400	-0.13323200
O	-0.51786600	-1.48299700	-1.25402700
O	-1.59602600	-0.74927100	1.18666900
O	-0.37742800	1.69754000	1.02066700
O	1.00929900	-0.78917700	1.05133500
O	1.09150100	0.75898800	-1.03630000
C	2.30656900	0.70388700	-0.28429200
C	2.31834300	-0.59726000	0.49837700
H	2.35713500	1.56910100	0.37593400

H	3.12543000	0.71978800	-1.00038200
H	2.56387500	-1.44605800	-0.13880900
H	3.00698000	-0.53249100	1.33782400
H	-1.15370900	-1.39411100	1.76659100
H	-0.77042400	1.55346600	1.89629000
O	-1.61109600	1.05905200	-0.79518400
H	-1.23952500	1.78315400	0.15405600

TS3_C



Thermochemistry:

Zero-point correction= 0.105549 (Hartree/Particle)
Thermal correction to Energy= 0.117325
Thermal correction to Enthalpy= 0.118269
Thermal correction to Gibbs Free Energy= 0.068327
Sum of electronic and zero-point Energies= -829.115392
Sum of electronic and thermal Energies= -829.103616
Sum of electronic and thermal Enthalpies= -829.102672
Sum of electronic and thermal Free Energies= -829.152614

Frequency: Infrared:

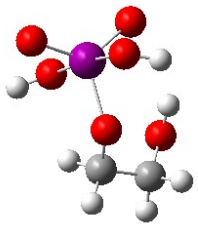
-744.52 2044.5382

Cartesian coordinates:

0 1

I	-0.42100300	-0.03050200	-0.08859100
O	-0.68664100	-0.64457200	-1.75454900
O	-1.63585900	-1.28289900	0.66541000
O	-0.55037100	0.63593900	1.83494800
O	1.27384100	-1.35598300	0.44426800
O	1.29252500	1.34181000	-0.46751100
C	2.46085100	0.93553400	-0.09172500
C	2.45283500	-0.96339400	0.08732900
H	2.77230100	1.22251200	0.91244700
H	3.21961900	0.89625900	-0.87303100
H	2.77721000	-1.25031500	-0.91248300
H	3.19808100	-0.93532800	0.88170200
H	-1.97190100	-1.81873000	-0.07532800
H	0.24841500	1.15886700	2.00464500
O	-1.64965600	1.38456000	-0.42524200
H	-1.76336200	1.87966700	0.40516100

IC2_B



Thermochemistry:

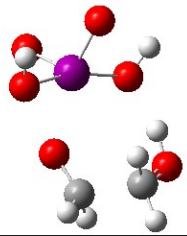
Zero-point correction= 0.110915 (Hartree/Particle)
Thermal correction to Energy= 0.122232
Thermal correction to Enthalpy= 0.123176
Thermal correction to Gibbs Free Energy= 0.073078
Sum of electronic and zero-point Energies= -829.137091
Sum of electronic and thermal Energies= -829.125774
Sum of electronic and thermal Enthalpies= -829.124830
Sum of electronic and thermal Free Energies= -829.174929

Cartesian coordinates:

0 1

I	0.72996200	-0.04920200	0.04275500
O	0.56524000	-0.27793600	1.78417700
O	1.36284300	1.75170800	0.21719200
O	-2.83373100	-0.35236300	1.04959600
O	-0.72992300	0.79236900	-0.81405600
C	-1.99195400	0.16295100	-1.18573500
C	-3.03484300	0.40827200	-0.13337500
H	-1.84741000	-0.89476600	-1.38148200
H	-2.26144400	0.66914700	-2.11255000
H	-3.08771300	1.47511000	0.09840800
H	-3.99672500	0.10063300	-0.54584500
H	-2.05063700	-0.01925100	1.50557700
H	0.78522100	2.23485200	0.83289100
O	2.14059500	-0.41111400	-0.95219000
O	-0.03340400	-1.78882100	-0.23589100
H	0.15855300	-2.09608400	-1.13897100

TS3_B



Thermochemistry:

Zero-point correction= 0.105025 (Hartree/Particle)
Thermal correction to Energy= 0.116815
Thermal correction to Enthalpy= 0.117759
Thermal correction to Gibbs Free Energy= 0.067176
Sum of electronic and zero-point Energies= -829.094440

Sum of electronic and thermal Energies=	-829.082650		
Sum of electronic and thermal Enthalpies=	-829.081706		
Sum of electronic and thermal Free Energies=	-829.132289		
Frequency:	**Infrared:**		
-898.12	11585.9187		
Cartesian coordinates:			
0 1			
I	-0.70589100	-0.05334300	-0.01718400
O	0.36699700	-1.70559800	0.54812500
O	-1.70233600	-0.99256100	-1.15604900
O	1.02612500	1.17358100	0.80551400
O	2.84116300	-1.11148900	-0.11003600
C	2.72907900	0.05284600	-0.74310000
C	2.19915100	1.35365400	0.26741800
H	1.88909500	0.11966500	-1.45422700
H	3.68112100	0.41531900	-1.11760800
H	3.00326000	1.18427300	0.99697500
H	2.29368700	2.21956600	-0.39089700
H	-0.05152000	-2.49595300	0.16802500
H	1.93606400	-1.47741900	0.10798300
O	-1.60268200	0.06043900	1.50279300
O	-1.28762800	1.68817600	-0.74209400
H	-2.04198600	1.52233200	-1.33143200

4. Topological analysis based on QTAIM.

Table S28. Calculated bond distances (d, Å), electronic charge densities at BCP (ρ, a.u.) for IC2_C and TS3_C structures.

Calculated at the B3PW91/6-311+G(2d,p) with 6-311+G(2d,p) basis set for C, O, H atoms and both: the full basis set (DGDZVP) for Iodine atom, the ϱ-BCP computed based on derived wave function.							
No.	**Bonds**	**ϱ-BCP$_{(IC2_C)}$ [a.u]**	**ϱ-BCP$_{(TS3_C)}$ [a.u]**	**Δϱ-BCP$_{(TS3_C-IC2_C)}$ [a.u]**	**d-Bond Dist.$_{(IC2\_C)}$ [Å]**	**d-Bond Dist.$_{(TS3\_C)}$ [Å]**	**Δd-Bond Dist.$_{(TS3\_C-IC2\_C)}$ [Å]**
1	I1 - O2	0.1800	0.1714	-0.0086	1.8265	1.8447	0.0183
2	I1 - O3	0.1403	0.1370	-0.0033	1.9550	1.9619	0.0069
3	I1 - O4	0.1328	0.1094	-0.0234	1.9877	2.0890	0.1013
4	I1 - O5	0.1309	0.0773	-0.0536	2.0009	2.2777	0.2768
5	I1 - O6	0.1302	0.0747	-0.0555	2.0020	2.2977	0.2957
6	C7 - C8	0.2520	0.0944	-0.1575	1.5185	1.9130	0.3945
7	O6 - C7	0.2435	0.3407	0.0972	1.4330	1.2904	-0.1426
8	O5 - C8	0.2449	0.3399	0.0950	1.4315	1.2913	-0.1403
9	C7 - H9	0.2856	0.2868	0.0012	1.0928	1.0929	0.0002
10	C7 - H10	0.2843	0.2827	-0.0015	1.0910	1.0938	0.0028
11	C8 - H11	0.2855	0.2872	0.0017	1.0930	1.0926	-0.0004
12	C8 - H12	0.2844	0.2832	-0.0012	1.0906	1.0932	0.0026
13	O3 - H13	0.3463	0.3458	-0.0004	0.9731	0.9742	0.0011
14	O4 - H14	0.3469	0.3507	0.0039	0.9723	0.9702	-0.0021
15	I1 - O15	0.1379	0.1354	-0.0025	1.9616	1.9668	0.0052
16	O15 - H16	0.3468	0.3457	-0.0012	0.9726	0.9742	0.0017

No.-sequence number; **ϱ-BCP** – electron density at Bond Critical Point; **Δϱ-BCP**$_{(TS3\_C\text{-}IC2\_C)}$ – electron density difference between corresponding two Bond Critical Points of the transition state structure TS3_C and intermediate structure IC2_C, **d-Bond Dist.** - Bond Distance between the atoms in Å; **Δd-Bond Dist.**$_{(TS3\_C\text{-}IC2\_C)}$ - difference between two corresponding bond distances of the transition state structure TS3_C and intermediate structure IC2_C.

Table S29. Calculated bond angles (∠,˚), in IC2_C and TS3_C structures .

Calculated at the B3PW91/6-311+G(2d,p) with 6-311+G(2d,p) basis set for C, O, H atoms and both: the full basis set (DGDZVP) for Iodine atom.				
No.	**Bond angles**	**∠$_{(IC2\_C)}$**	**∠$_{(TS3\_C)}$**	**Δ∠ $_{(TS3\_C\text{-}IC2\_C)}$ [Å]**
1	O2 - I1 - O3	94.73130	92.85459	-1.87671
2	O2 - I1 - O4	171.96741	166.69954	-5.26787
3	O2 - I1 - O5	95.97872	98.20327	2.22455
4	O2 - I1 - O6	96.22805	98.77491	2.54686
5	O2 - I1 - O15	89.45495	89.20521	-0.24974
6	O3 - I1 - O4	78.66853	77.96563	-0.70290
7	O3 - I1 - O5	89.50017	90.45620	0.95603
8	O3 - I1 - O6	167.82450	164.73701	-3.08749
9	O3 - I1 - O15	96.50361	98.23218	1.72857
10	O4 - I1 - O5	88.59623	91.54337	2.94714
11	O4 - I1 - O6	90.79583	92.04150	1.24567
12	O4 - I1 - O15	86.78094	82.70268	-4.07826
13	O5 - I1 - O6	84.10446	78.17794	-5.92652
14	O5 - I1 - O15	171.55847	168.31043	-3.24804
15	O6 - I1 - O15	88.89810	91.81331	2.91521
16	I1 - O2 - O3	44.42689	45.25003	0.82314
17	I1 - O2 - O4	4.18635	7.06498	2.87863
18	I1 - O2 - O5	44.36123	46.09646	1.73523
19	I1 - O2 - O6	44.24063	45.96918	1.72855
20	I1 - O2 - O15	47.33500	47.25772	-0.07728
21	I1 - O3 - O2	40.84180	41.89538	1.05358
22	I1 - O3 - O4	51.24538	53.23682	1.99144
23	I1 - O3 - O5	45.92015	48.99833	3.07818
24	I1 - O3 - O6	6.16033	8.23667	2.07634

25	I1 - O3 - O15	41.83412	40.94613	-0.88799
26	I1 - O4 - O2	3.84624	6.23548	2.38924
27	I1 - O4 - O3	50.08609	48.79755	-1.28854
28	I1 - O4 - O5	45.89602	46.63759	0.74157
29	I1 - O4 - O6	44.80471	46.60832	1.80361
30	I1 - O4 - O15	46.20888	46.68896	0.48008
31	I1 - O5 - O2	39.66005	35.70027	-3.95978
32	I1 - O5 - O3	44.57968	40.54547	-4.03421
33	I1 - O5 - O4	45.50776	41.81904	-3.68872
34	I1 - O5 - O6	47.96554	51.21921	3.25367
35	I1 - O5 - O15	4.17884	5.41521	1.23637
36	I1 - O6 - O2	39.53132	35.25591	-4.27541
37	I1 - O6 - O3	6.01518	7.02631	1.01113
38	I1 - O6 - O4	44.39946	41.35019	-3.04927
39	I1 - O6 - O5	47.93000	50.60285	2.67285
40	I1 - O6 - O15	44.95542	39.79452	-5.16090
41	I1 - O15 - O2	43.21005	43.53707	0.32702
42	I1 - O15 - O3	41.66227	40.82170	-0.84057
43	I1 - O15 - O4	47.01018	50.60836	3.59818
44	I1 - O15 - O5	4.26270	6.27435	2.01165
45	I1 - O15 - O6	46.14648	48.39217	2.24569
46	C7 - O6 - O5	66.12253	62.98997	-3.13256
47	C8 - O5 - O3	155.97756	152.21622	-3.76135
48	H9 - C7 - O6	116.98791	109.35147	-7.63644
49	H10 - C7 - O6	115.67908	106.56712	-9.11196
50	H11 - C8 - O5	117.03873	109.83144	-7.20729
51	H12 - C8 - O5	115.47222	106.57544	-8.89677
52	H13 - O3 - I1	104.55563	105.01691	0.46128
53	H14 - O4 - O3	146.60387	157.11699	10.51313
54	H16 - O15 -O2	148.76456	150.31855	1.55398

55	I1-O5-C8	108.64835	115.83204	7.18369
56	O5-C8-C7	108.75013	109.48057	0.73044
57	C8-C7-O6	109.10543	109.78573	0.68030
58	C7-O6-I1	110.57135	116.12607	5.55472
59	O5-I1-O6	84.10446	78.17794	-5.92652

Table S30. Calculated electron density derivatives for TS3_C structure.

Calculated at the B3PW91/6-311+G(2d,p) with 6-311+G(2d,p) basis set for C, O, H atoms and both: the full basis set (DGDZVP) for Iodine atom, the ϱ-BCP computed based on derived wave function.						
No.	**Bonds**	**DelSqRho [Rho]**	**Ellipticity**	**K**	**BPL - GBL_I**	**L**
1	I1 - O2	0.416944	0.011607	0.105122	0.000059	-0.104236
2	I1 - O3	0.259293	0.097343	0.070032	0.000685	-0.064823
3	I1 - O4	0.190308	0.084258	0.043532	0.002605	-0.047577
4	I1 - O5	0.140193	0.075646	0.016972	0.010594	-0.035048
5	I1 - O6	0.137329	0.066936	0.015291	0.009453	-0.034332
6	C7 - C8	0.004129	0.020815	0.033859	0.00351	-0.001032
7	O6 - C7	-0.447502	0.030053	0.564012	0.000208	0.111876
8	O5 - C8	-0.44523	0.027214	0.56214	0.000237	0.111308
9	C7 - H9	-1.013866	0.024882	0.283433	0.00041	0.253467
10	C7 - H10	-0.991826	0.033153	0.278643	0.00042	0.247957
11	C8 - H11	-1.016989	0.024382	0.28406	0.000427	0.254247
12	C8 - H12	-0.996039	0.031915	0.279484	0.00041	0.24901
13	O3 - H13	-2.398265	0.017454	0.663558	0.000472	0.599566
14	O4 - H14	-2.356663	0.015581	0.660279	0.000229	0.589166
15	I1 - O15	0.258137	0.096211	0.068292	0.000884	-0.064534
16	O15 - H16	-2.401528	0.017175	0.664561	0.000391	0.600382

No.-sequence number; **DelSqRho [Rho]** - Laplacian of the electron density (DelSqRho) [Rho]; **Ellipticity** - Ellipticity of the electron dencity at BCPs; **K** - Hamiltonian form of the electronic kinetic energy density at BCPs (K); **BPL - GBL_I** - Bond Path Length (BPL) with a corresponding Geometric Bond Length (GBL_I, the Euclidean distance between nuclear attractors connected by a Bond Path) (BPL - GBL_I); **L** - Electronic Lagrangian density at BCPs.

Table S31. Calculated electron density derivatives for IC2_C structure.

Calculated at the B3PW91/6-311+G(2d,p) with 6-311+G(2d,p) basis set for C, O, H atoms and both: the full basis set (DGDZVP) for Iodine atom, the ϱ-BCP computed based on derived wave function.

No.	Bonds	DelSqRho [Rho]	Ellipticity	K	BPL - GBL_I	L
1	I1 - O2	0.402356	0.009071	0.115659	0.00003	-0.100589
2	I1 - O3	0.257998	0.082829	0.07378	0.000715	-0.064499
3	I1 - O4	0.223887	0.087497	0.06661	0.001506	-0.055972
4	I1 - O5	0.203807	0.079519	0.065097	0.001547	-0.050952
5	I1 - O6	0.206242	0.076937	0.064232	0.00186	-0.051561
6	C7 - C8	-0.48804	0.029432	0.326286	0.001137	0.12201
7	O6 - C7	-0.494326	0.031066	0.32903	0.001042	0.123581
8	O5 - C8	-0.572613	0.034805	0.19971	0.000521	0.143153
9	C7 - H9	-0.995042	0.039392	0.281685	0.000437	0.248761
10	C7 - H10	-0.997131	0.03404	0.281664	0.000353	0.249283
11	C8 - H11	-0.993329	0.039548	0.281275	0.000447	0.248332
12	C8 - H12	-0.998844	0.033286	0.282053	0.000351	0.249711
13	O3 - H13	-2.408921	0.017507	0.666199	0.00043	0.60223
14	O4 - H14	-2.396828	0.017807	0.664527	0.000407	0.599207
15	I1 - O15	0.255883	0.072993	0.071172	0.001136	-0.063971
16	O15 - H16	-2.40848	0.017186	0.666615	0.000425	0.60212

No.-sequence number; **DelSqRho [Rho]** - Laplacian of the electron density (DelSqRho) [Rho]; **Ellipticity** - Ellipticity of the electron dencity at BCPs; **K** - Hamiltonian form of the electronic kinetic energy density at BCPs (K); **BPL - GBL_I** - Bond Path Length (BPL) with a corresponding Geometric Bond Length (GBL_I, the Euclidean distance between nuclear attractors connected by a Bond Path) (BPL - GBL_I); **L** - Electronic Lagrangian density at BCPs.

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