Supporting Information

Ab Initio Path-Integral Calculations of Kinetic and Equilibrium Isotope Effects on Base-Catalyzed RNA Transphosphorylation Models

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ab initio, path integral, kinetic isotope effects, equilibrium isotope effects, biocatalysis, RNA, transphosphorylation, Bigeleisen equation, anharmonicity, quantum tunneling

Contents

Native LTS in Solution	4 processors, 4GB Memory Computing Time (hh:mm:ss)[b]			4 processors, 100GB Memory Computing Time (hh:mm:ss)[b]		
Electronic Struct. Theory	Energy	Force	Frequency	Energy	Force	Frequency
HF/3-21+G*	00:00:09	00:00:13	00:01:07	00:00:10	00:00:12	00:01:07
B3LYP/6-31+G(d)	00:00:34	00:00:42	00:04:35	00:00:33	00:00:41	00:04:32
M06-2X/6-31+G(d)	00:00:48	00:00:57	00:06:32	00:00:49	00:00:57	00:06:19
B3LYP/6-311+G(d,p)	00:01:17	00:01:34	00:11:25	00:01:09	00:01:23	00:07:49
M06-2X/6-311+G(d,p)	00:01:26	00:01:45	00:17:35	00:01:18	00:01:36	00:10:44
MP2/6-311+G(d,p)	00:01:19	00:04:04	02:10:38	00:01:58	00:03:21	01:55:36
CCSD/6-311+G(d,p)	01:51:14	--[c]	--[c]	01:26:43	--[c]	--[c]
CCSD(T)/6-311+G(d,p)	04:54:00	--[c]	--[c]	04:18:35	--[c]	--[c]

(A)

Native LTS in Solution	8 processors, 4GB Memory Computing Time (hh:mm:ss)[b]			8 processors, 100GB Memory Computing Time (hh:mm:ss)[b]		
Electronic Struct. Theory	Energy	Force	Frequency	Energy	Force	Frequency
HF/3-21+G*	00:00:08	00:00:10	00:00:43	00:00:08	00:00:10	00:00:37
B3LYP/6-31+G(d)	00:00:24	00:00:28	00:02:42	00:00:23	00:00:27	00:02:20
M06-2X/6-31+G(d)	00:00:31	00:00:37	00:03:32	00:00:32	00:00:36	00:03:39
B3LYP/6-311+G(d,p)	00:00:43	00:00:51	00:06:08	00:00:52	00:01:00	00:04:33
M06-2X/6-311+G(d,p)	00:00:47	00:00:59	00:10:07	00:00:56	00:01:07	00:05:44
MP2/6-311+G(d,p)	00:00:45	00:03:31	01:16:46	00:01:48	00:02:49	01:10:24
CCSD/6-311+G(d,p)	01:22:41	--[c]	--[c]	01:01:58	--[c]	--[c]
CCSD(T)/6-311+G(d,p)	02:45:59	--[c]	--[c]	02:36:46	--[c]	--[c]

(B)

Native LTS in Solution	16 processors, 4GB Memory Computing Time (hh:mm:ss)[b]			16 processors, 100GB Memory Computing Time (hh:mm:ss)[b]		
Electronic Struct. Theory	Energy	Force	Frequency	Energy	Force	Frequency
HF/3-21+G*	00:00:07	00:00:09	00:00:34	00:00:08	00:00:09	00:00:32
B3LYP/6-31+G(d)	00:00:19	00:00:22	00:01:29	00:00:18	00:00:22	00:01:21
M06-2X/6-31+G(d)	00:00:24	00:00:27	00:02:11	00:00:24	00:00:27	00:02:10
B3LYP/6-311+G(d,p)	00:00:26	00:00:32	00:02:54	00:00:44	00:00:49	00:02:33
M06-2X/6-311+G(d,p)	00:00:29	00:00:34	00:04:29	00:00:46	00:00:51	00:03:41
MP2/6-311+G(d,p)	00:00:29	00:05:23	00:51:09	00:01:45	00:02:37	00:44:07
CCSD/6-311+G(d,p)	01:01:03	--[c]	--[c]	00:55:59	--[c]	--[c]
CCSD(T)/6-311+G(d,p)	02:02:32	--[c]	--[c]	01:44:31	--[c]	--[c]

(C)

Table S1. Computing times of single-point energy, force, and frequency calculations at the eight levels of electronic structure theory.[a]

[a] The number of basis functions in this table for 3-21+G*, 6-31+G(d), and 6-311+G(d,p) are 141, 189, and 248, respectively. All calculations were performed with (A) four, (B) eight, (C) sixteen processors of Intel Xeon E7-4870 2.40GHz, sharing 4GB or 100GB memory of 1066MHz quad ranked LV RDIMMs, on a single-compute-node machine (jiraiya) that has forty processors of Intel Xeon E7-4870 2.40GHz (4×10C), sharing 1TB memory of 1066MHz quad ranked LV RDIMMs (64×16GB). The LTS structures are the optimized structures in solution respectively for each level of theory, except for CCSD and CCSD(T) single-point energy calculations. In these CCSD and CCSD(T) calculations, we used the optimized structure in solution at the MP2/6-311+G(d,p) level.

[b] hh = hours in two digits, mm = minutes in two digits, ss = seconds in two digits.

[c] The calculation was not performed us.

Native (37°C)	Gas (kcal/mol)			Solution (kcal/mol)		
Electronic Struct. Theory CCSD/6-311+G(d,p) //	$\Delta G^{\ddagger}_{ETS}$	ΔG_{Int}	$\Delta G^{\ddagger}_{LTS}$	$\Delta G^{\ddagger}_{ETS}$	ΔG_{Int}	$\Delta G^{\ddagger}_{LTS}$
HF/3-21+G*	--	--	42.6	19.3	19.2	21.9
B3LYP/6-31+G(d)	--	--	43.3	19.4	18.9	22.1
M06-2X/6-31+G(d)	--	--	42.8	18.6	19.0	21.5
B3LYP/6-311+G(d,p)	--	--	43.5	19.2[b]	--[c]	22.0
M06-2X/6-311+G(d,p)	--	--	43.1	18.8	18.9	21.6
MP2/6-311+G(d,p)	--	--	43.0	19.4	19.4	22.1

(A)

S3′ (37°C)	Gas (kcal/mol)			Solution (kcal/mol)		
Electronic Struct. Theory CCSD/6-311+G(d,p) //	$\Delta G^{\ddagger}_{ETS}$	ΔG_{Int}	$\Delta G^{\ddagger}_{LTS}$	$\Delta G^{\ddagger}_{ETS}$	ΔG_{Int}	$\Delta G^{\ddagger}_{LTS}$
HF/3-21+G*	34.2	--[c]	35.3	17.6	16.4	17.8
B3LYP/6-31+G(d)	34.7	33.6	35.6	16.9	15.5	17.4
M06-2X/6-31+G(d)	34.9	34.4	35.3	16.5	15.4	16.5
B3LYP/6-311+G(d,p)	34.7	33.7	35.9	16.9	15.6	17.6
M06-2X/6-311+G(d,p)	34.2	33.8	34.9	16.0[d]	14.9[d]	16.1[d]
MP2/6-311+G(d,p)	34.3	33.6	34.9	17.2	16.1	17.8

(B)

S5′ (37°C)	Gas (kcal/mol)			Solution (kcal/mol)		
Electronic Struct. Theory CCSD/6-311+G(d,p) //	$\Delta G^{\ddagger}_{ETS}$	ΔG_{Int}	$\Delta G^{\ddagger}_{LTS}$	$\Delta G^{\ddagger}_{ETS}$	ΔG_{Int}	$\Delta G^{\ddagger}_{LTS}$
HF/3-21+G*	27.6	--	--	17.1	--	--
B3LYP/6-31+G(d)	28.4	--	--	18.0	--	--
M06-2X/6-31+G(d)	28.8	--	--	16.7	--	--
B3LYP/6-311+G(d,p)	28.5	--	--	18.1	--	--
M06-2X/6-311+G(d,p)	28.3	--	--	17.1	--	--
MP2/6-311+G(d,p)	28.5	--	--	17.2	--	--

(C)

Table S2. Dual-level CCSD relative free energy calculated for stationary points along the intrinsic reaction coordinate of the (A) native, (B) S3′, and (C) S5′ simplest models of RNA transphosphorylation in both gas and solution phases.[a]

[a] CCSD is not included in the thermal corrections. "--" denotes the molecular structure of that particular state could not be determined by us.

[b] As in Table 2, the ETS is determined but along with very small value of non-reactive imaginary frequency.

[c] As in Table 2, no intermediate could be determined by us that satisfies all default criteria in GAUSSIAN 09.[41]

[d] As in Table 2, the reactant is determined but along with very small value of non-reactive imaginary frequency.

	Root-Mean-Square Deviation (RMSD)		
Electronic Struct. Theory	Gas (kcal/mol)	Solution (kcal/mol)	All (kcal/mol)
HF/3-21+G*	11.2	5.4	8.0
B3LYP/6-31+G(d)	1.8	1.6	1.7
M06-2X/6-31+G(d)	1.6	2.4	2.1
B3LYP/6-311+G(d,p)	1.3	1.4	1.3
M06-2X/6-311+G(d,p)	1.6	2.5	2.2
MP2/6-311+G(d,p)	0.2	0.2	0.2

Table S3. Root-mean-square deviations between single-level calculations, and their respective counterparts of dual-level calculations that have single-point energy of CCSD(T)/6-311+G(d,p), for all native, S3′, and S5′ reactions.

	Root-Mean-Square Deviation (RMSD)		
Electronic Struct. Theory	Gas (kcal/mol)	Solution (kcal/mol)	All (kcal/mol)
HF/3-21+G*	11.0	5.4	7.9
B3LYP/6-31+G(d)	1.9	1.2	1.5
M06-2X/6-31+G(d)	1.3	2.9	2.4
B3LYP/6-311+G(d,p)	1.4	1.0	1.2
M06-2X/6-311+G(d,p)	1.5	3.2	2.6
MP2/6-311+G(d,p)	0.2	0.2	0.2

Table S4. Root-mean-square deviations between single-level calculations and CCSD(T)/6-311+G(d,p)//MP2/6-311+G(d,p), for all native, S3′, and S5′ reactions.

Electronic Struct. Theory	Root-Mean-Square Deviation (RMSD)		
CCSD(T)/6-311+G(d,p) //	Gas (kcal/mol)	Solution (kcal/mol)	All (kcal/mol)
HF/3-21+G*	0.5	0.3	0.4
B3LYP/6-31+G(d)	0.3	0.5	0.4
M06-2X/6-31+G(d)	0.6	0.6	0.6
B3LYP/6-311+G(d,p)	0.4	0.5	0.5
M06-2X/6-311+G(d,p)	0.2	0.9	0.7
MP2/6-311+G(d,p)	0	0	0

Table S5. Root-mean-square deviations between the dual-level calculations at the CCSD(T)/6-311+G(d,p)//MP2/6-311+G(d,p) level and other dual-level calculations with single-point energy of CCSD(T)/6-311+G(d,p) , for all native, S3′, and S5′ reactions.

	Root-Mean-Square Deviation (RMSD)		
Electronic Struct. Theory	Gas (kcal/mol)	Solution (kcal/mol)	All (kcal/mol)
HF/3-21+G*	9.5	3.9	6.5
B3LYP/6-31+G(d)	1.2	0.8	1.0
M06-2X/6-31+G(d)	2.7	3.9	3.4
B3LYP/6-311+G(d,p)	1.7	0.9	1.4
M06-2X/6-311+G(d,p)	2.9	4.0	3.5
MP2/6-311+G(d,p)	1.8	1.7	1.7

Table S6. Root-mean-square deviations between single-level calculations and their respective counterparts of dual-level calculations that have single-point energy of CCSD/6-311+G(d,p) , for all native, S3′, and S5′ reactions.

Electronic Struct. Theory	Root-Mean-Square Deviation (RMSD)		
CCSD/6-311+G(d,p) //	Gas (kcal/mol)	Solution (kcal/mol)	All (kcal/mol)
HF/3-21+G*	1.8	1.7	1.7
B3LYP/6-31+G(d)	2.2	1.6	1.9
M06-2X/6-31+G(d)	2.3	1.0	1.7
B3LYP/6-311+G(d,p)	2.4	1.6	2.0
M06-2X/6-311+G(d,p)	1.9	1.0	1.5
MP2/6-311+G(d,p)	1.9	1.7	1.8

Table S7. Root-mean-square deviations between the dual-level calculations at the CCSD(T)/6-311+G(d,p)//MP2/6-311+G(d,p) level and other dual-level calculations with single-point energy of CCSD/6-311+G(d,p) , for all native, S3′, and S5′ reactions.

Native	Gas (Å)						Solution (Å)					
Electronic Struct. Theory	ETS		Int		LTS		ETS		Int		LTS	
CCSD/6-311+G(d,p) //	$BO_{O5'}$	$BO_{O2'}$	$BO_{O5'}$	$BO_{O2'}$	$BO_{O5'}$	$BO_{O2'}$	$BO_{O5'}$	$BO_{O2'}$	$BO_{O5'}$	$BO_{O2'}$	$BO_{O5'}$	$BO_{O2'}$
HF/3-21+G*	--	--	--	--	0.09	0.45	0.51	0.25	0.47	0.40	0.16	0.52
B3LYP/6-31+G(d)	--	--	--	--	0.11	0.42	0.48	0.26	0.45	0.38	0.16	0.50
M06-2X/6-31+G(d)	--	--	--	--	0.10	0.44	0.52	0.17	0.45	0.41	0.13	0.52
B3LYP/6-311+G(d,p)	--	--	--	--	0.11	0.42	0.47[b]	0.30[b]	--[c]	--[c]	0.17	0.50
M06-2X/6-311+G(d,p)	--	--	--	--	0.09	0.44	0.51	0.18	0.45	0.39	0.12	0.52
MP2/6-311+G(d,p)	--	--	--	--	0.10	0.43	0.49	0.24	0.45	0.38	0.15	0.51

(A)

S3′	Gas (Å)						Solution (Å)					
Electronic Struct. Theory	ETS		Int		LTS		ETS		Int		LTS	
CCSD/6-311+G(d,p) //	$BO_{O5'}$	$BO_{O2'}$	$BO_{O5'}$	$BO_{O2'}$	$BO_{O5'}$	$BO_{O2'}$	$BO_{O5'}$	$BO_{O2'}$	$BO_{O5'}$	$BO_{O2'}$	$BO_{O5'}$	$BO_{O2'}$
HF/3-21+G*	0.47	0.13	--[c]	--[c]	0.12	0.48	0.52	0.16	0.44	0.44	0.15	0.53
B3LYP/6-31+G(d)	0.44	0.18	0.40	0.39	0.15	0.44	0.49	0.18	0.42	0.40	0.16	0.50
M06-2X/6-31+G(d)	0.47	0.11	0.42	0.42	0.09	0.47	0.52	0.13	0.43	0.42	0.11	0.52
B3LYP/6-311+G(d,p)	0.43	0.19	0.39	0.38	0.16	0.43	0.49	0.18	0.41	0.39	0.17	0.49
M06-2X/6-311+G(d,p)	0.47	0.11	0.41	0.41	0.09	0.47	0.52	0.13	0.42	0.42	0.11	0.52
MP2/6-311+G(d,p)	0.45	0.14	0.40	0.40	0.13	0.45	0.50	0.15	0.42	0.41	0.15	0.50

(B)

S5′	Gas (Å)						Solution (Å)					
Electronic Struct. Theory	ETS		Int		LTS		ETS		Int		LTS	
CCSD/6-311+G(d,p) //	$BO_{S5'}$	$BO_{O2'}$	$BO_{S5'}$	$BO_{O2'}$	$BO_{S5'}$	$BO_{O2'}$	$BO_{S5'}$	$BO_{O2'}$	$BO_{S5'}$	$BO_{O2'}$	$BO_{S5'}$	$BO_{O2'}$
HF/3-21+G*	0.45	0.14	--	--	--	--	0.66	0.18	--	--	--	--
B3LYP/6-31+G(d)	0.37	0.15	--	--	--	--	0.62	0.18	--	--	--	--
M06-2X/6-31+G(d)	0.47	0.13	--	--	--	--	0.64	0.15	--	--	--	--
B3LYP/6-311+G(d,p)	0.35	0.14	--	--	--	--	0.61	0.18	--	--	--	--
M06-2X/6-311+G(d,p)	0.46	0.13	--	--	--	--	0.63	0.15	--	--	--	--
MP2/6-311+G(d,p)	0.41	0.16	--	--	--	--	0.65	0.17	--	--	--	--

(C)

Table S8. Dual-level CCSD Wiberg bond order (bond index) for stationary points along the intrinsic reaction coordinate of the (A) native, (B) S3′, and (C) S5′ simplest models of RNA transphosphorylation in both gas and solution phases.[a]

[a] $BO_{O5'}$ is the bond order between O5′ and P, $BO_{O2'}$ is the bond order between O2′ and P, $BO_{S5'}$ is the bond order between S5′ and P. "--" denotes the molecular structure of that particular state could not be determined us.
[b] As in Table 2, the ETS is determined but along with very small value of non-reactive imaginary frequency.
[c] As in Table 2, no minimum point could be determined by us that satisfies all default criteria in GAUSSIAN 09.[41]

Native (37°C)	Equilibrium Isotope Effects in Gas (ratio of isotopic equilibrium constants) Nucleophile (2′-OH) deprotonation				
Electronic Struct. Theory	$^{18}E_{Nuc}$	$^{18}E_{Lea}$	$^{18}E_{O3'}$	$^{18}E_{O1P}$	$^{18}E_{O2P}$
HF/3-21+G*	1.0386	1.0048	0.9995	1.0010	1.0029
B3LYP/6-31+G(d)	1.0287	1.0054	1.0017	1.0017	1.0021
M06-2X/6-31+G(d)	1.0295	1.0044	1.0009	1.0013	1.0020
B3LYP/6-311+G(d,p)	1.0292	1.0058	1.0016	1.0015	1.0021
M06-2X/6-311+G(d,p)	1.0304	1.0055	1.0010	1.0012	1.0022
MP2/6-311+G(d,p)	1.0310	1.0059	1.0008	1.0017	1.0023

(A)

S3′ (37°C)	Equilibrium Isotope Effects in Gas (ratio of isotopic equilibrium constants) Nucleophile (2′-OH) deprotonation				
Electronic Struct. Theory	$^{18}E_{Nuc}$	$^{18}E_{Lea}$	$^{34}E_{S3'}$	$^{18}E_{O1P}$	$^{18}E_{O2P}$
HF/3-21+G*	1.0383	1.0014	1.0003	1.0020	1.0019
B3LYP/6-31+G(d)	1.0281	1.0027	1.0007	1.0028	1.0014
M06-2X/6-31+G(d)	1.0289	1.0024	1.0002	1.0021	1.0025
B3LYP/6-311+G(d,p)	1.0286	1.0028	1.0008	1.0028	1.0013
M06-2X/6-311+G(d,p)	1.0298	1.0028	1.0004	1.0022	1.0022
MP2/6-311+G(d,p)	1.0299	1.0026	1.0004	1.0023	1.0016

(B)

S5′ (37°C)	Equilibrium Isotope Effects in Gas (ratio of isotopic equilibrium constants) Nucleophile (2′-OH) deprotonation				
Electronic Struct. Theory	$^{18}E_{Nuc}$	$^{34}E_{Lea}$	$^{18}E_{O3'}$	$^{18}E_{O1P}$	$^{18}E_{O2P}$
HF/3-21+G*	1.0383	1.0018	0.9987	1.0007	1.0021
B3LYP/6-31+G(d)	1.0282	1.0016	1.0000	1.0011	1.0011
M06-2X/6-31+G(d)	1.0293	1.0015	0.9987	1.0012	1.0013
B3LYP/6-311+G(d,p)	1.0288	1.0016	0.9998	1.0009	1.0010
M06-2X/6-311+G(d,p)	1.0299	1.0014	0.9988	1.0013	1.0014
MP2/6-311+G(d,p)	1.0306	1.0016	0.9994	1.0008	1.0007

(C)

Table S9. Equilibrium isotope effects on nucleophile (2′-OH) deprotonation of the (A) native, (B) S3′, and (C) S5′ simplest models of RNA transphosphorylation in the gas phase.[a]
[a] All values are computed from the Bigeleisen equation.

Native (37°C)	Equilibrium Isotope Effects in Gas (ratio of isotopic equilibrium constants) Nucleophile (2′-OH) deprotonation				
Electronic Struct. Theory MP2/6-311+G(d,p) //	$^{18}E_{Nuc}$	$^{18}E_{Lea}$	$^{18}E_{O3'}$	$^{18}E_{O1P}$	$^{18}E_{O2P}$
HF/3-21+G*	1.0357	1.0050	1.0005	1.0017	1.0026
B3LYP/6-31+G(d)	1.0297	1.0058	1.0010	1.0017	1.0018
M06-2X/6-31+G(d)	1.0302	1.0051	1.0008	1.0019	1.0019
B3LYP/6-311+G(d,p)	1.0294	1.0060	1.0009	1.0016	1.0020
M06-2X/6-311+G(d,p)	1.0300	1.0054	1.0007	1.0018	1.0021
MP2/6-311+G(d,p)	1.0310	1.0059	1.0008	1.0017	1.0023

(A)

S3′ (37°C)	Equilibrium Isotope Effects in Gas (ratio of isotopic equilibrium constants) Nucleophile (2′-OH) deprotonation				
Electronic Struct. Theory MP2/6-311+G(d,p) //	$^{18}E_{Nuc}$	$^{18}E_{Lea}$	$^{34}E_{S3'}$	$^{18}E_{O1P}$	$^{18}E_{O2P}$
HF/3-21+G*	1.0348	1.0019	1.0004	1.0022	1.0015
B3LYP/6-31+G(d)	1.0290	1.0031	1.0004	1.0025	1.0011
M06-2X/6-31+G(d)	1.0292	1.0026	1.0003	1.0024	1.0011
B3LYP/6-311+G(d,p)	1.0288	1.0030	1.0004	1.0025	1.0013
M06-2X/6-311+G(d,p)	1.0294	1.0033	1.0002	1.0037	1.0026
MP2/6-311+G(d,p)	1.0299	1.0026	1.0004	1.0023	1.0016

(B)

S5′ (37°C)	Equilibrium Isotope Effects in Gas (ratio of isotopic equilibrium constants) Nucleophile (2′-OH) deprotonation				
Electronic Struct. Theory MP2/6-311+G(d,p) //	$^{18}E_{Nuc}$	$^{34}E_{Lea}$	$^{18}E_{O3'}$	$^{18}E_{O1P}$	$^{18}E_{O2P}$
HF/3-21+G*	1.0353	1.0014	0.9994	1.0010	1.0015
B3LYP/6-31+G(d)	1.0293	1.0016	0.9996	1.0009	1.0005
M06-2X/6-31+G(d)	1.0298	1.0015	0.9989	1.0010	1.0005
B3LYP/6-311+G(d,p)	1.0291	1.0017	0.9994	1.0008	1.0006
M06-2X/6-311+G(d,p)	1.0296	1.0015	0.9989	1.0009	1.0006
MP2/6-311+G(d,p)	1.0306	1.0016	0.9994	1.0008	1.0007

(C)

Table S10. Dual-level MP2 equilibrium isotope effects on nucleophile (2′-OH) deprotonation of the (A) native, (B) S3′, and (C) S5′ simplest models of RNA transphosphorylation in the gas phase.[a]
[a] All values are computed from the Bigeleisen equation.

Native (37°C)	Equilibrium Isotope Effects in Solution (ratio of isotopic equilibrium constants) Nucleophile (2′-OH) deprotonation				
Electronic Struct. Theory MP2/6-311+G(d,p) //	$^{18}E_{Nuc}$	$^{18}E_{Lea}$	$^{18}E_{O3'}$	$^{18}E_{O1P}$	$^{18}E_{O2P}$
HF/3-21+G*	1.0241	1.0022	0.9990	0.9996	1.0002
B3LYP/6-31+G(d)	1.0220	1.0007	1.0010	0.9999	1.0009
M06-2X/6-31+G(d)	1.0216	1.0015	0.9983	1.0002	1.0004
B3LYP/6-311+G(d,p)	1.0225	1.0006	1.0010	0.9997	1.0011
M06-2X/6-311+G(d,p)	1.0224	1.0017	0.9982	1.0002	1.0005
MP2/6-311+G(d,p)	1.0218	1.0020	0.9984	1.0004	1.0003

(A)

S3′ (37°C)	Equilibrium Isotope Effects in Solution (ratio of isotopic equilibrium constants) Nucleophile (2′-OH) deprotonation				
Electronic Struct. Theory MP2/6-311+G(d,p) //	$^{18}E_{Nuc}$	$^{18}E_{Lea}$	$^{34}E_{S3'}$	$^{18}E_{O1P}$	$^{18}E_{O2P}$
HF/3-21+G*	1.0258	1.0005	1.0001	1.0002	0.9999
B3LYP/6-31+G(d)	1.0206	1.0006	1.0002	1.0007	1.0006
M06-2X/6-31+G(d)	1.0245	1.0004	1.0006	1.0007	1.0001
B3LYP/6-311+G(d,p)	1.0213	1.0006	1.0002	1.0007	1.0006
M06-2X/6-311+G(d,p)	1.0254[b]	1.0003[b]	1.0006[b]	1.0006[b]	1.0002[b]
MP2/6-311+G(d,p)	1.0271	1.0001	1.0007	1.0004	1.0004

(B)

S5′ (37°C)	Equilibrium Isotope Effects in Solution (ratio of isotopic equilibrium constants) Nucleophile (2′-OH) deprotonation				
Electronic Struct. Theory MP2/6-311+G(d,p) //	$^{18}E_{Nuc}$	$^{34}E_{Lea}$	$^{18}E_{O3'}$	$^{18}E_{O1P}$	$^{18}E_{O2P}$
HF/3-21+G*	1.0255	0.9999	1.0007	1.0006	1.0010
B3LYP/6-31+G(d)	1.0208	1.0002	1.0022	1.0010	1.0004
M06-2X/6-31+G(d)	1.0215	0.9994	1.0018	1.0006	1.0009
B3LYP/6-311+G(d,p)	1.0218	1.0002	1.0023	1.0011	1.0004
M06-2X/6-311+G(d,p)	1.0223	0.9994	1.0016	1.0006	1.0011
MP2/6-311+G(d,p)	1.0225	0.9999	1.0002	1.0004	1.0001

(C)

Table S11. Dual-level MP2 equilibrium isotope effects on nucleophile (2′-OH) deprotonation of the (A) native, (B) S3′, and (C) S5′ simplest models of RNA transphosphorylation in solution.[a]
[a] All values are computed from the Bigeleisen equation.
[b] As in Table 2, the ground state after deprotonation is determined but along with very small value of non-reactive imaginary frequency.

Native (37°C)	Kinetic Isotope Effects in Gas (ratio of isotopic reaction rates)									
Electronic Struct. Theory	ETS					LTS				
	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$
HF/3-21+G*	--	--	--	--	--	0.9534	1.0918	1.0080	1.0021	1.0010
B3LYP/6-31+G(d)	--	--	--	--	--	0.9755	1.0599	1.0064	1.0022	1.0014
M06-2X/6-31+G(d)	--	--	--	--	--	0.9686	1.0710	1.0025	1.0012	1.0003
B3LYP/6-311+G(d,p)	--	--	--	--	--	0.9764	1.0599	1.0069	1.0022	1.0011
M06-2X/6-311+G(d,p)	--	--	--	--	--	0.9691	1.0720	1.0026	1.0011	0.9999
MP2/6-311+G(d,p)	--	--	--	--	--	0.9727	1.0669	1.0084	1.0011	0.9999

(A)

S3′ (37°C)	Kinetic Isotope Effects in Gas (ratio of isotopic reaction rates)									
Electronic Struct. Theory	ETS					LTS				
	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{34}k_{S3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{34}k_{S3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$
HF/3-21+G*	1.0255	1.0106	1.0016	1.0012	1.0019	0.9531	1.0751	1.0033	1.0024	1.0024
B3LYP/6-31+G(d)	1.0229	1.0105	1.0024	1.0014	1.0021	0.9769	1.0523	1.0042	1.0016	1.0018
M06-2X/6-31+G(d)	1.0274	1.0094	1.0016	1.0006	1.0010	0.9700	1.0658	1.0032	1.0017	1.0011
B3LYP/6-311+G(d,p)	1.0221	1.0114	1.0024	1.0013	1.0018	0.9776	1.0518	1.0041	1.0014	1.0017
M06-2X/6-311+G(d,p)	1.0282	1.0093	1.0014	1.0002	1.0009	0.9700	1.0662	1.0030	1.0012	1.0015
MP2/6-311+G(d,p)	1.0250	1.0115	1.0024	1.0009	1.0008	0.9738	1.0591	1.0041	1.0013	1.0009

(B)

S5′ (37°C)	Kinetic Isotope Effects in Gas (ratio of isotopic reaction rates)									
Electronic Struct. Theory	ETS					LTS				
	$^{18}k_{Nuc}$	$^{34}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$	$^{18}k_{Nuc}$	$^{34}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$
HF/3-21+G*	1.0103	1.0065	1.0008	1.0010	1.0010	--	--	--	--	--
B3LYP/6-31+G(d)	1.0123	1.0054	1.0012	1.0007	1.0010	--	--	--	--	--
M06-2X/6-31+G(d)	1.0196	1.0038	1.0025	1.0001	1.0008	--	--	--	--	--
B3LYP/6-311+G(d,p)	1.0114	1.0056	1.0015	1.0005	1.0008	--	--	--	--	--
M06-2X/6-311+G(d,p)	1.0191	1.0037	1.0030	1.0001	1.0008	--	--	--	--	--
MP2/6-311+G(d,p)	1.0117	1.0051	1.0030	1.0002	1.0010	--	--	--	--	--

(C)

Table S12. Kinetic isotope effects on the (A) native, (B) S3′, and (C) S5′ simplest models of RNA transphosphorylation in the gas phase.[a]
[a] All values are computed from the Bigeleisen equation. "--" denotes the molecular structure of that particular state could not be determined by us.

Native (37°C)	Kinetic Isotope Effects in Gas (ratio of isotopic reaction rates)									
Electronic Struct. Theory	ETS					LTS				
MP2/6-311+G(d,p) //	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$
HF/3-21+G*	--	--	--	--	--	0.9619	1.0726	1.0083	1.0015	0.9996
B3LYP/6-31+G(d)	--	--	--	--	--	0.9752	1.0609	1.0076	1.0019	1.0008
M06-2X/6-31+G(d)	--	--	--	--	--	0.9708	1.0686	1.0037	1.0009	0.9994
B3LYP/6-311+G(d,p)	--	--	--	--	--	0.9760	1.0616	1.0075	1.0016	1.0004
M06-2X/6-311+G(d,p)	--	--	--	--	--	0.9711	1.0691	1.0035	1.0008	0.9990
MP2/6-311+G(d,p)	--	--	--	--	--	0.9727	1.0669	1.0084	1.0011	0.9999

(A)

S3′ (37°C)	Kinetic Isotope Effects in Gas (ratio of isotopic reaction rates)									
Electronic Struct. Theory	ETS					LTS				
MP2/6-311+G(d,p) //	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{34}k_{S3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{34}k_{S3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$
HF/3-21+G*	1.0210	1.0109	1.0019	1.0015	1.0015	0.9626	1.0606	1.0049	1.0034	1.0022
B3LYP/6-31+G(d)	1.0215	1.0110	1.0027	1.0018	1.0019	0.9763	1.0547	1.0039	1.0017	1.0016
M06-2X/6-31+G(d)	1.0281	1.0097	1.0022	1.0006	1.0008	0.9715	1.0616	1.0044	1.0017	1.0017
B3LYP/6-311+G(d,p)	1.0212	1.0120	1.0029	1.0018	1.0016	0.9769	1.0555	1.0036	1.0014	1.0013
M06-2X/6-311+G(d,p)	1.0288	1.0103	1.0022	1.0005	1.0005	0.9708	1.0527	1.0038	1.0014	1.0013
MP2/6-311+G(d,p)	1.0250	1.0115	1.0024	1.0009	1.0008	0.9738	1.0591	1.0041	1.0013	1.0009

(B)

S5′ (37°C)	Kinetic Isotope Effects in Gas (ratio of isotopic reaction rates)									
Electronic Struct. Theory	ETS					LTS				
MP2/6-311+G(d,p) //	$^{18}k_{Nuc}$	$^{34}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$	$^{18}k_{Nuc}$	$^{34}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$
HF/3-21+G*	1.0116	1.0050	1.0016	1.0003	1.0004	--	--	--	--	--
B3LYP/6-31+G(d)	1.0110	1.0059	1.0021	1.0006	1.0009	--	--	--	--	--
M06-2X/6-31+G(d)	1.0188	1.0036	1.0034	1.0005	1.0009	--	--	--	--	--
B3LYP/6-311+G(d,p)	1.0097	1.0062	1.0019	1.0002	1.0006	--	--	--	--	--
M06-2X/6-311+G(d,p)	1.0174	1.0038	1.0034	1.0002	1.0008	--	--	--	--	--
MP2/6-311+G(d,p)	1.0117	1.0051	1.0030	1.0002	1.0010	--	--	--	--	--

(C)

Table S13. Dual-level MP2 kinetic isotope effects on the (A) native, (B) S3′, and (C) S5′ simplest models of RNA transphosphorylation in the gas phase.[a]
[a] All values are computed from the Bigeleisen equation. "--" denotes the molecular structure of that particular state could not be determined by us.

Native (37°C) Electronic Struct. Theory	Kinetic Isotope Effects in Solution (ratio of isotopic reaction rates)									
	ETS					LTS				
MP2/6-311+G(d,p) //	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$
HF/3-21+G*	1.0096	1.0069	1.0028	1.0048	1.0055	0.9590	1.0716	1.0026	1.0044	1.0036
B3LYP/6-31+G(d)	1.0158	1.0065	1.0062	1.0047	1.0041	0.9667	1.0614	1.0062	1.0052	1.0027
M06-2X/6-31+G(d)	1.0244	1.0055	1.0042	1.0043	1.0032	0.9647	1.0714	1.0064	1.0043	1.0028
B3LYP/6-311+G(d,p)	1.0118[b]	1.0081[b]	1.0071[b]	1.0054[b]	1.0047[b]	0.9670	1.0612	1.0063	1.0051	1.0024
M06-2X/6-311+G(d,p)	1.0230	1.0060	1.0045	1.0045	1.0034	0.9649	1.0714	1.0065	1.0043	1.0026
MP2/6-311+G(d,p)	1.0190	1.0075	1.0046	1.0047	1.0045	0.9665	1.0683	1.0043	1.0039	1.0029

(A)

S3′ (37°C) Electronic Struct. Theory	Kinetic Isotope Effects in Solution (ratio of isotopic reaction rates)									
	ETS					LTS				
MP2/6-311+G(d,p) //	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{34}k_{S3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{34}k_{S3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$
HF/3-21+G*	1.0184	1.0084	1.0011	1.0036	1.0025	0.9585	1.0605	1.0016	1.0033	1.0017
B3LYP/6-31+G(d)	1.0239	1.0086	1.0013	1.0036	1.0038	0.9700	1.0592	1.0013	1.0020	1.0026
M06-2X/6-31+G(d)	1.0281	1.0074	1.0013	1.0024	1.0020	0.9655	1.0709	1.0014	1.0014	1.0018
B3LYP/6-311+G(d,p)	1.0232	1.0093	1.0013	1.0036	1.0037	0.9702	1.0583	1.0014	1.0018	1.0021
M06-2X/6-311+G(d,p)	1.0284[c]	1.0078[c]	1.0013[c]	1.0028[c]	1.0019[c]	0.9652[c]	1.0722[c]	1.0014[c]	1.0014[c]	1.0017[c]
MP2/6-311+G(d,p)	1.0264	1.0088	1.0011	1.0035	1.0030	0.9659	1.0666	1.0013	1.0020	1.0024

(B)

S5′ (37°C) Electronic Struct. Theory	Kinetic Isotope Effects in Solution (ratio of isotopic reaction rates)									
	ETS					LTS				
MP2/6-311+G(d,p) //	$^{18}k_{Nuc}$	$^{34}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$	$^{18}k_{Nuc}$	$^{34}k_{Lea}$	$^{18}k_{O3'}$	$^{18}k_{O1P}$	$^{18}k_{O2P}$
HF/3-21+G*	1.0158	1.0023	1.0038	1.0034	1.0039	--	--	--	--	--
B3LYP/6-31+G(d)	1.0191	1.0021	1.0052	1.0043	1.0041	--	--	--	--	--
M06-2X/6-31+G(d)	1.0218	1.0022	1.0044	1.0037	1.0031	--	--	--	--	--
B3LYP/6-311+G(d,p)	1.0174	1.0022	1.0055	1.0043	1.0041	--	--	--	--	--
M06-2X/6-311+G(d,p)	1.0204	1.0022	1.0047	1.0034	1.0031	--	--	--	--	--
MP2/6-311+G(d,p)	1.0211	1.0019	1.0064	1.0037	1.0040	--	--	--	--	--

(C)

Table S14. Dual-level MP2 kinetic isotope effects on the (A) native, (B) S3′, and (C) S5′ simplest models of RNA transphosphorylation in solution.[a]

[a] All values are computed from the Bigeleisen equation. "--" denotes the molecular structure of that particular state could not be determined by us.
[b] As in Table 2, the ETS is determined but along with very small value of non-reactive imaginary frequency.
[c] As in Table 2, the reactant is determined but along with very small value of non-reactive imaginary frequency.

Native (37°C) Electronic Struct. Theory	*Ab Initio* Path-Integral Calculations Equilibrium Isotope Effects in Gas Nucleophile (2′-OH) deprotonation	
MP2/6-311+G(d,p)	$^{18}E_{Nuc}$	$^{18}E_{Lea}$
Full Harmonic	1.0310	1.0059
Partial Harmonic	1.0297	1.0055
Partial KP1/P20	1.0319	1.0057
Partial KP2/P20	1.0317	1.0058
Full Harmonic × Partial(KP1/Harmonic)	1.0332	1.0061
Full Harmonic × Partial(KP2/Harmonic)	1.0330	1.0061

(A)

S3′ (37°C) Electronic Struct. Theory	*Ab Initio* Path-Integral Calculations Equilibrium Isotope Effects in Gas Nucleophile (2′-OH) deprotonation	
MP2/6-311+G(d,p)	$^{18}E_{Nuc}$	$^{18}E_{Lea}$
Full Harmonic	1.0299	1.0026
Partial Harmonic	1.0282	1.0022
Partial KP1/P20	1.0180	1.0010
Partial KP2/P20	1.0179	1.0010
Full Harmonic × Partial(KP1/Harmonic)	1.0197	1.0014
Full Harmonic × Partial(KP2/Harmonic)	1.0196	1.0014

(B)

S5′ (37°C) Electronic Struct. Theory	*Ab Initio* Path-Integral Calculations Equilibrium Isotope Effects in Gas Nucleophile (2′-OH) deprotonation	
MP2/6-311+G(d,p)	$^{18}E_{Nuc}$	$^{34}E_{Lea}$
Full Harmonic	1.0306	1.0016
Partial Harmonic	1.0292	1.0016
Partial KP1/P20	1.0221	1.0016
Partial KP2/P20	1.0220	1.0016
Full Harmonic × Partial(KP1/Harmonic)	1.0235	1.0015
Full Harmonic × Partial(KP2/Harmonic)	1.0234	1.0015

(C)

Table S15. *Ab initio* path-integral calculations of equilibrium isotope effects on nucleophile (2′-OH) deprotonation of the (A) native, (B) S3′, and (C) S5′ simplest models of RNA transphosphorylation in the gas phase.[a]
[a] "Full Harmonic" is the value computed from the Bigeleisen equation, in which the entire system is quantized. "Partial" means only six or seven nuclei are further quantized to compute the anharmonicity, which is excluded in the Bigeleisen equation. See Computational Details for the meanings of the notations of KP1/KP2 and P20.

Native (37°C)	*Ab Initio* Path-Integral Calculations Kinetic Isotope Effects in Gas			
Electronic Struct. Theory	ETS		LTS	
MP2/6-311+G(d,p)	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{18}k_{Nuc}$	$^{18}k_{Lea}$
Full Harmonic	--	--	0.9727	1.0669
Partial Harmonic	--	--	0.9738	1.0646
Partial KP1/P20	--	--	0.9751	1.0654
Partial KP2/P20	--	--	0.9751	1.0653
Full Harmonic × Partial(KP1/Harmonic)	--	--	0.9740	1.0677
Full Harmonic × Partial(KP2/Harmonic)	--	--	0.9739	1.0676

(A)

S3′ (37°C)	*Ab Initio* Path-Integral Calculations Kinetic Isotope Effects in Gas			
Electronic Struct. Theory	ETS		LTS	
MP2/6-311+G(d,p)	$^{18}k_{Nuc}$	$^{18}k_{Lea}$	$^{18}k_{Nuc}$	$^{18}k_{Lea}$
Full Harmonic	1.0250	1.0115	0.9738	1.0591
Partial Harmonic	1.0256	1.0110	0.9756	1.0570
Partial KP1/P20	1.0259	1.0113	0.9756	1.0568
Partial KP2/P20	1.0259	1.0113	0.9756	1.0568
Full Harmonic × Partial(KP1/Harmonic)	1.0253	1.0118	0.9738	1.0588
Full Harmonic × Partial(KP2/Harmonic)	1.0253	1.0118	0.9738	1.0589

(B)

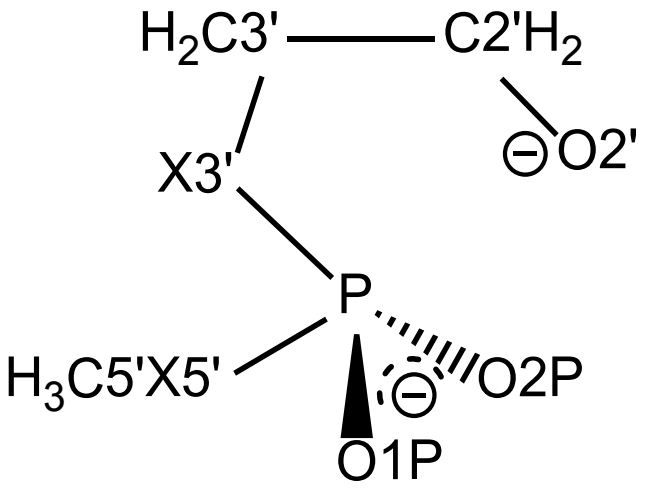
S5′ (37°C)	*Ab Initio* Path-Integral Calculations Kinetic Isotope Effects in Gas			
Electronic Struct. Theory	ETS		LTS	
MP2/6-311+G(d,p)	$^{18}k_{Nuc}$	$^{34}k_{Lea}$	$^{18}k_{Nuc}$	$^{34}k_{Lea}$
Full Harmonic	1.0117	1.0051	--	--
Partial Harmonic	1.0131	1.0053	--	--
Partial KP1/P20	1.0141	1.0053	--	--
Partial KP2/P20	1.0141	1.0053	--	--
Full Harmonic × Partial(KP1/Harmonic)	1.0127	1.0051	--	--
Full Harmonic × Partial(KP2/Harmonic)	1.0127	1.0051	--	--

(C)

Table S16. *Ab initio* path-integral calculations of kinetic isotope effects on the (A) native, (B) S3′, and (C) S5′ simplest models of RNA transphosphorylation in the gas phase.[a]

[a] "Full Harmonic" is the value computed from the Bigeleisen equation, in which the entire system is quantized. "Partial" means only six nuclei are further quantized to compute the anharmonicity and tunneling effects, which are excluded in the Bigeleisen equation. See Computational Details for the meanings of the notations of KP1/KP2 and P20. "--" denotes the molecular structure of that particular state could not be determined by us.

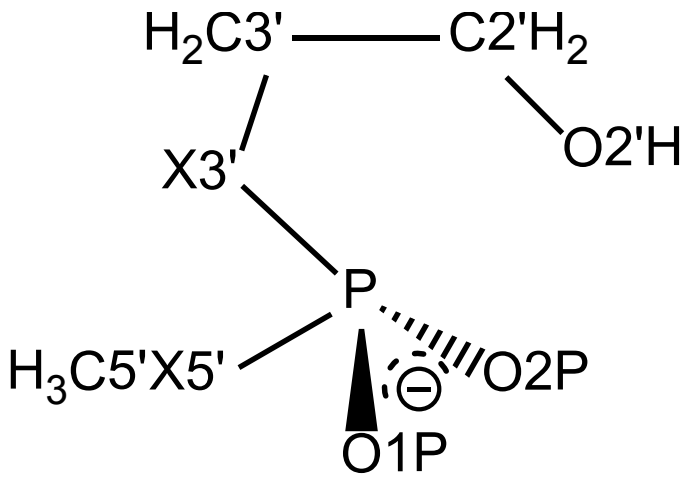
Atomic Radii Used for Building up Dianionic Molecular Cavities in PCM Calculations:



Atomic numberings in a model for base-catalyzed RNA transphosphorylation, in which X is either oxygen or sulfur.

Center for spherical cavity	Radius of cavity (Å)	Scaling factor
P	1.913	1.100
O1P	1.568	1.100
O2P	1.568	1.100
C2′	1.703	1.100
C3′ when X3′=O3′	1.703	1.100
C3′ when X3′=S3′	1.793	1.100
C5′ when X5′=O5′	1.883	1.100
C5′ when X5′=S5′	1.973	1.100
O2′	1.485	1.100
O3′	1.568	1.100
O5′	1.485	1.100
S3′	2.108	1.100
S5′	1.990	1.100

Atomic Radii Used for Building up Anionic Molecular Cavities in PCM Calculations:



Atomic numberings in a model for base-catalyzed RNA transphosphorylation, in which X is either oxygen or sulfur.

Center for spherical cavity	Radius of cavity (Å)	Scaling factor
P	1.947	1.100
O1P	1.602	1.100
O2P	1.602	1.100
C2′	1.737	1.100
C3′ when X3′=O3′	1.737	1.100
C3′ when X3′=S3′	1.827	1.100
C5′ when X5′=O5′	1.917	1.100
C5′ when X5′=S5′	2.007	1.100
O2′	1.557	1.100
O3′	1.602	1.100
O5′	1.602	1.100
S3′	2.142	1.100
S5′	2.142	1.100

Native Dianionic Reactant Structure at the Gas-HF/3-21+G* level:

C	-1.466702	2.126849	-0.131299
O	-1.460960	0.848661	-0.797303
P	-1.168525	-0.534968	0.050348
O	-1.254678	-1.658533	-0.931866
O	0.345665	-0.274626	0.516554
C	1.567712	-0.317073	-0.313812
C	2.760803	0.192813	0.508963
O	3.948289	0.192649	-0.265849
O	-2.041256	-0.489265	1.270004
H	1.727378	-1.337142	-0.632079
H	1.419545	0.309328	-1.184236
H	2.490096	1.194822	0.875636
H	2.831235	-0.445178	1.401250
H	-1.676295	2.871963	-0.889221
H	-2.230441	2.144535	0.636982
H	-0.501012	2.319565	0.321023

Native Early Transition State (ETS) Structure at the Gas-HF/3-21+G* level:

P	0.097548	-0.696409	0.028054
O	0.135527	0.830996	-0.642375
C	1.355755	1.573455	-0.486801
C	2.272030	0.696299	0.394534
H	1.131200	2.535532	-0.039621
H	1.794511	1.724122	-1.468760
H	2.113318	0.908554	1.447069
O	1.847683	-0.630800	0.080086
O	-0.218397	-0.630125	1.492034
O	-0.110619	-1.836928	-0.903420
O	-2.358352	-0.140118	-0.396327
C	-2.833359	1.004918	0.267035
H	-2.489003	1.952960	-0.192159
H	-2.521226	1.047750	1.322515
H	3.321873	0.815113	0.146535
H	-3.947173	1.069868	0.275016

Native Dianionic Reactant Structure at the Gas-B3LYP/6-31+G(d) level:

C	-1.389455	2.107090	-0.113381
O	-1.419780	0.895467	-0.839693
P	-1.176566	-0.534112	0.047750
O	-1.254541	-1.637568	-0.979337
O	0.353475	-0.297304	0.603138
C	1.513242	-0.301034	-0.275927
C	2.788001	0.163579	0.482306
O	3.902109	0.161210	-0.291547
O	-2.086050	-0.478284	1.258488
H	1.663816	-1.315817	-0.666675
H	1.332178	0.371330	-1.126334
H	2.520296	1.178587	0.911728
H	2.850456	-0.505156	1.393257
H	-1.592458	2.923698	-0.823909
H	-2.152655	2.117350	0.679969
H	-0.405585	2.275708	0.349333

Native Early Transition State (ETS) Structure at the Gas-B3LYP/6-31+G(d) level:

P	0.040882	-0.670714	0.013979
O	0.157103	0.956073	-0.539768
C	1.446567	1.512207	-0.481584
C	2.292325	0.610110	0.430728
H	1.378913	2.551615	-0.109916
H	1.893923	1.538447	-1.496763
H	2.111732	0.873131	1.495328
O	1.876139	-0.680714	0.135857
O	-0.326399	-0.751890	1.479921
O	-0.125447	-1.727304	-1.046119
O	-2.305705	-0.017840	-0.483835
C	-2.825709	0.933794	0.311328
H	-2.430063	1.984403	0.128400
H	-2.667806	0.762804	1.412663
H	3.374870	0.732581	0.226850
H	-3.959425	1.054472	0.202478

Native Dianionic Reactant Structure at the Gas-M06-2X/6-31+G(d) level:

C	-1.102081	2.109180	-0.117689
O	-1.310673	0.925413	-0.846735
P	-1.209569	-0.494402	0.042969
O	-1.330226	-1.598022	-0.964770
O	0.308933	-0.353542	0.627304
C	1.439477	-0.340008	-0.263906
C	2.724240	0.072156	0.490218
O	3.822984	0.088748	-0.292923
O	-2.136358	-0.361754	1.221641
H	1.569861	-1.337607	-0.703341
H	1.257985	0.372257	-1.082792
H	2.469541	1.067571	0.964778
H	2.783028	-0.633726	1.369279
H	-1.251429	2.953569	-0.804766
H	-1.812060	2.187342	0.718061
H	-0.080485	2.151913	0.286379

Native Early Transition State (ETS) Structure at the Gas-M06-2X/6-31+G(d) level:

P	0.105982	-0.701740	0.058838
O	0.097996	0.722277	-0.845967
C	1.085753	1.592876	-0.378351
C	2.221204	0.721247	0.256677
H	0.664082	2.288846	0.365151
H	1.454194	2.179997	-1.235590
H	2.281508	0.923160	1.341651
O	1.888421	-0.598785	0.001034
O	-0.135376	-0.415583	1.516035
O	-0.126618	-1.960906	-0.706158
O	-2.335866	-0.218334	-0.314305
C	-2.644138	0.978329	0.203600
H	-2.270813	1.868118	-0.393270
H	-2.242702	1.150632	1.239227
H	3.202844	0.955932	-0.193662
H	-3.764212	1.175361	0.297256

Native Dianionic Reactant Structure at the Gas-B3LYP/6-311+G(d,p) level:

C	-1.335830	2.120081	-0.124884
O	-1.396731	0.902941	-0.838948
P	-1.186254	-0.527623	0.049224
O	-1.285829	-1.629255	-0.969041
O	0.345875	-0.321368	0.601952
C	1.514715	-0.354128	-0.264537
C	2.772002	0.185020	0.470035
O	3.894000	0.140797	-0.284358
O	-2.092121	-0.446792	1.253894
H	1.694317	-1.385987	-0.586340
H	1.329521	0.254724	-1.157553
H	2.481331	1.221726	0.819763
H	2.826300	-0.409064	1.429259
H	-1.532124	2.933439	-0.836266
H	-2.086458	2.149415	0.676796
H	-0.345951	2.273670	0.324319

Native Early Transition State (ETS) Structure at the Gas-B3LYP/6-311+G(d,p) level:

P	0.041864	-0.678359	0.014274
O	0.149682	0.950488	-0.528046
C	1.433328	1.517496	-0.479601
C	2.294117	0.621290	0.423161
H	1.361494	2.552071	-0.104072
H	1.872161	1.548972	-1.495560
H	2.120643	0.886477	1.486382
O	1.885141	-0.670827	0.136358
O	-0.321894	-0.767441	1.473232
O	-0.115903	-1.721476	-1.049772
O	-2.316756	-0.029017	-0.471113
C	-2.822172	0.942106	0.305111
H	-2.385854	1.974725	0.130338
H	-2.695781	0.776183	1.410423
H	3.370508	0.754980	0.208882
H	-3.944936	1.102812	0.172197

Native Dianionic Reactant Structure at the Gas-M06-2X/6-311+G(d,p) level:

C	-0.957926	2.122757	-0.128625
O	-1.267867	0.949919	-0.841064
P	-1.233082	-0.472520	0.043542
O	-1.403865	-1.566486	-0.959640
O	0.288163	-0.401760	0.625729
C	1.427067	-0.415359	-0.256305
C	2.695267	0.067247	0.482291
O	3.803508	0.044297	-0.284576
O	-2.150442	-0.300769	1.217751
H	1.584012	-1.432156	-0.632667
H	1.238064	0.239584	-1.116606
H	2.418458	1.085692	0.882008
H	2.747140	-0.571778	1.406997
H	-1.127882	2.974532	-0.796539
H	-1.596210	2.220155	0.758541
H	0.090220	2.122289	0.195364

Native Early Transition State (ETS) Structure at the Gas-M06-2X/6-311+G(d,p) level:

P	0.105479	-0.702779	0.058149
O	0.113044	0.708644	-0.860947
C	1.093671	1.587079	-0.393983
C	2.221857	0.724793	0.267043
H	0.662665	2.286500	0.336399
H	1.472078	2.161537	-1.251168
H	2.263067	0.942652	1.346866
O	1.890810	-0.598187	0.027934
O	-0.155380	-0.401416	1.503361
O	-0.117924	-1.962175	-0.695563
O	-2.341181	-0.205397	-0.339012
C	-2.651204	0.972946	0.219583
H	-2.123441	1.862438	-0.235503
H	-2.411530	1.044023	1.313207
H	3.205471	0.953331	-0.173544
H	-3.751380	1.250542	0.149468

Native Dianionic Reactant Structure at the Gas-MP2/6-311+G(d,p) level:

C	-1.083847	2.127311	-0.141104
O	-1.280568	0.929829	-0.865200
P	-1.215544	-0.489577	0.045608
O	-1.355104	-1.600394	-0.955412
O	0.307510	-0.383454	0.646836
C	1.458894	-0.449965	-0.227436
C	2.698837	0.157980	0.464796
O	3.828026	0.068483	-0.286458
O	-2.147365	-0.323528	1.219070
H	1.662615	-1.497239	-0.481149
H	1.257878	0.098400	-1.156389
H	2.393078	1.211157	0.726974
H	2.753306	-0.364463	1.460464
H	-1.130881	2.955852	-0.859010
H	-1.861644	2.261873	0.623000
H	-0.104478	2.138632	0.353755

Native Early Transition State (ETS) Structure at the Gas-MP2/6-311+G(d,p) level:

P	0.068287	-0.695486	0.028388
O	0.107314	0.880119	-0.635217
C	1.344638	1.528562	-0.508028
C	2.214531	0.675321	0.423376
H	1.189635	2.549458	-0.121064
H	1.832157	1.595720	-1.498235
H	1.969567	0.908380	1.475861
O	1.884765	-0.635254	0.098917
O	-0.264168	-0.663526	1.495396
O	-0.112383	-1.812568	-0.948033
O	-2.329048	-0.088097	-0.440384
C	-2.724895	0.970810	0.294860
H	-2.255456	1.956251	-0.001122
H	-2.504377	0.882658	1.391973
H	3.287923	0.864912	0.253597
H	-3.841236	1.181372	0.246483

Native Dianionic Reactant Structure at the PCM-HF/3-21+G* level:

C	-1.633440	2.146071	-0.081749
O	-1.507003	0.830750	-0.730298
P	-1.128781	-0.533736	0.033466
O	-1.170171	-1.623079	-1.002821
O	0.370734	-0.284207	0.523855
C	1.573751	-0.223527	-0.344250
C	2.750764	0.198378	0.530142
O	3.946259	0.248828	-0.272165
O	-1.978596	-0.675164	1.267271
H	1.731281	-1.214142	-0.771223
H	1.389417	0.502935	-1.137897
H	2.521955	1.174846	0.974608
H	2.847931	-0.521692	1.352100
H	-1.848742	2.846391	-0.875131
H	-2.444821	2.116777	0.634433
H	-0.701537	2.398375	0.409531

Native Early Transition State (ETS) Structure at the PCM-HF/3-21+G* level:

P	-0.314144	-0.509648	-0.046480
O	0.270861	0.953139	-0.480680
C	1.681234	1.352614	-0.480967
C	2.378005	0.382981	0.467248
H	1.716963	2.395326	-0.167913
H	2.052832	1.247201	-1.501154
H	2.229721	0.695398	1.507400
O	1.728925	-0.870771	0.201502
O	-0.501701	-0.729956	1.455322
O	-0.310078	-1.652875	-1.059297
O	-1.888568	0.026967	-0.420607
C	-2.551451	1.105124	0.289405
H	-1.994319	2.029160	0.184360
H	-2.652082	0.861355	1.341213
H	3.450804	0.341363	0.261875
H	-3.533999	1.218577	-0.152622

Native Intermediate Structure at the PCM-HF/3-21+G* level:

P	-0.239331	-0.525216	-0.034648
O	0.278989	0.973512	-0.530800
C	1.684614	1.370093	-0.457263
C	2.318187	0.337110	0.472144
H	1.725141	2.391490	-0.081056
H	2.104210	1.316867	-1.462709
H	2.180316	0.615681	1.521104
O	1.577212	-0.860997	0.158715
O	-0.500171	-0.677766	1.476083
O	-0.353136	-1.704392	-1.019026
O	-1.852596	0.037903	-0.428139
C	-2.499313	1.127899	0.269274
H	-1.926703	2.044067	0.171780
H	-2.618012	0.893430	1.322030
H	3.379474	0.194338	0.267650
H	-3.477781	1.265683	-0.178662

Native Late Transition State (LTS) Structure at the PCM-HF/3-21+G* level:

P	0.010864	-0.615410	-0.005946
O	0.176338	0.969686	-0.356924
C	1.551501	1.498366	-0.445326
C	2.363037	0.535869	0.417606
H	1.535103	2.521330	-0.075149
H	1.858332	1.464347	-1.491480
H	2.290438	0.786943	1.478041
O	1.702380	-0.743175	0.167881
O	-0.441353	-0.925383	1.408377
O	-0.187347	-1.590143	-1.149132
O	-2.161356	-0.026372	-0.446111
C	-2.770628	1.047089	0.291612
H	-2.404056	2.021737	-0.037199
H	-2.563373	0.965714	1.361334
H	3.404391	0.462492	0.110110
H	-3.856538	1.043735	0.167454

Native Dianionic Reactant Structure at the PCM-B3LYP/6-31+G(d) level:

C	2.539359	1.656687	-0.105811
O	1.286611	1.036546	-0.450446
P	0.995066	-0.514419	0.055565
O	1.152856	-0.586919	1.565199
O	-0.565868	-0.626423	-0.396384
C	-1.617069	0.067241	0.345280
C	-2.920827	0.009558	-0.464805
O	-3.968867	0.632887	0.208752
O	1.770373	-1.488764	-0.813932
H	-1.747379	-0.432932	1.325356
H	-1.313324	1.120351	0.511135
H	-2.705953	0.477830	-1.462347
H	-3.124726	-1.074046	-0.677657
H	2.521817	2.661230	-0.542996
H	2.649206	1.732174	0.984513
H	3.384745	1.092148	-0.524967

Native Early Transition State (ETS) Structure at the PCM-B3LYP/6-31+G(d) level:

P	-0.298024	-0.518395	-0.043980
O	0.250822	1.022456	-0.453278
C	1.652800	1.348046	-0.472162
C	2.358413	0.377295	0.466204
H	1.746454	2.410594	-0.170386
H	2.025472	1.226522	-1.511416
H	2.200340	0.702855	1.527275
O	1.784789	-0.869735	0.206406
O	-0.514370	-0.790319	1.457890
O	-0.293384	-1.619074	-1.119973
O	-1.925936	0.041911	-0.450483
C	-2.544083	1.065021	0.317303
H	-2.025659	2.030600	0.205066
H	-2.574728	0.807038	1.387257
H	3.456243	0.394234	0.274446
H	-3.575907	1.179992	-0.045110

Native Intermediate Structure at the PCM-B3LYP/6-31+G(d) level:

P	-0.235671	-0.534429	-0.031697
O	0.259107	1.025643	-0.517478
C	1.651040	1.374210	-0.449026
C	2.306063	0.347844	0.468812
H	1.726609	2.414841	-0.074374
H	2.079977	1.320979	-1.472252
H	2.151786	0.631319	1.538934
O	1.661551	-0.862457	0.154460
O	-0.498347	-0.732771	1.481836
O	-0.334073	-1.683678	-1.063692
O	-1.903409	0.047913	-0.452171
C	-2.500975	1.091521	0.295943
H	-1.967308	2.048751	0.173560
H	-2.537700	0.854055	1.371595
H	3.399220	0.282702	0.283889
H	-3.532916	1.225140	-0.063909

Native Late Transition State (LTS) Structure at the PCM-B3LYP/6-31+G(d) level:

P	0.000617	-0.611310	-0.005399
O	0.168286	1.019325	-0.371890
C	1.536596	1.482658	-0.444520
C	2.335315	0.522805	0.425308
H	1.559515	2.530259	-0.086764
H	1.872203	1.439899	-1.502242
H	2.229938	0.779982	1.504005
O	1.754683	-0.750880	0.150283
O	-0.427312	-0.916065	1.432983
O	-0.187440	-1.599926	-1.157434
O	-2.175037	-0.005032	-0.468353
C	-2.758859	0.998261	0.303043
H	-2.343289	2.008871	0.093523
H	-2.627745	0.831998	1.395288
H	3.410563	0.505909	0.159014
H	-3.854190	1.071018	0.130461

Native Dianionic Reactant Structure at the PCM-M06-2X/6-31+G(d) level:

C	-1.189002	2.141000	-0.085269
O	-1.349115	0.913869	-0.802539
P	-1.180790	-0.487958	0.028270
O	-1.252687	-1.575209	-1.011641
O	0.320935	-0.358008	0.636367
C	1.441207	-0.300845	-0.272525
C	2.696254	0.087234	0.510825
O	3.812912	0.119158	-0.305302
O	-2.108229	-0.500525	1.216339
H	1.574788	-1.294302	-0.746264
H	1.238201	0.452247	-1.063432
H	2.479076	1.074167	0.997257
H	2.788978	-0.648791	1.351582
H	-1.374319	2.951694	-0.796459
H	-1.909179	2.202982	0.740790
H	-0.166980	2.222767	0.308499

Native Early Transition State (ETS) Structure at the PCM-M06-2X/6-31+G(d) level:

P	-0.350889	-0.512289	-0.048938
O	0.232031	0.975368	-0.476244
C	1.619298	1.319083	-0.510297
C	2.349841	0.415525	0.467802
H	1.691454	2.396961	-0.266951
H	1.994129	1.146485	-1.540547
H	2.124950	0.760973	1.510828
O	1.881439	-0.862095	0.224009
O	-0.484231	-0.757232	1.450663
O	-0.285068	-1.624897	-1.085942
O	-1.937954	0.015959	-0.428907
C	-2.507426	1.069524	0.324332
H	-1.974729	2.016005	0.153262
H	-2.492907	0.843432	1.399588
H	3.449315	0.531496	0.317841
H	-3.548889	1.187368	0.000400

Native Intermediate Structure at the PCM-M06-2X/6-31+G(d) level:

P	-0.225705	-0.532260	-0.027851
O	0.263086	0.991588	-0.583827
C	1.635351	1.354335	-0.467078
C	2.249816	0.338574	0.485854
H	1.695265	2.397469	-0.100598
H	2.108583	1.287648	-1.468389
H	2.047359	0.627790	1.543771
O	1.607239	-0.858741	0.150309
O	-0.483707	-0.642475	1.487716
O	-0.350684	-1.717163	-1.004163
O	-1.875835	0.039002	-0.449616
C	-2.434118	1.097900	0.287841
H	-1.828511	2.014912	0.214826
H	-2.536308	0.839980	1.352955
H	3.346409	0.260092	0.346638
H	-3.434312	1.313459	-0.114483

Native Late Transition State (LTS) Structure at the PCM-M06-2X/6-31+G(d) level:

P	0.044759	-0.630821	0.005323
O	0.127167	0.963503	-0.446447
C	1.458898	1.500345	-0.462330
C	2.276895	0.569098	0.419391
H	1.419422	2.539991	-0.087266
H	1.834974	1.487717	-1.505581
H	2.117145	0.796843	1.496627
O	1.762986	-0.715156	0.101788
O	-0.356399	-0.841830	1.453969
O	-0.193121	-1.657710	-1.083814
O	-2.234493	-0.083248	-0.406644
C	-2.693280	1.028433	0.276436
H	-2.297459	1.983451	-0.130594
H	-2.408025	1.017249	1.351218
H	3.358117	0.605179	0.190036
H	-3.799766	1.120167	0.253929

Native Dianionic Reactant Structure at the PCM-B3LYP/6-311+G(d,p) level:

C	2.520396	1.675392	-0.104818
O	1.282532	1.029623	-0.455340
P	0.997619	-0.518075	0.053429
O	1.168590	-0.586687	1.556859
O	-0.563713	-0.633949	-0.381650
C	-1.618382	0.060856	0.354608
C	-2.914318	0.012447	-0.464406
O	-3.964177	0.634575	0.203783
O	1.763853	-1.489279	-0.817769
H	-1.759792	-0.441911	1.330855
H	-1.312504	1.111468	0.527044
H	-2.687712	0.483302	-1.456900
H	-3.116740	-1.068541	-0.686291
H	2.494148	2.671433	-0.554853
H	2.616231	1.768231	0.983422
H	3.379236	1.120713	-0.504071

Native Early Transition State (ETS) Structure at the PCM-B3LYP/6-311+G(d,p) level:

P	-0.276851	-0.527307	-0.038657
O	0.253306	1.020793	-0.468330
C	1.651427	1.358476	-0.462013
C	2.341218	0.367177	0.465031
H	1.740859	2.411791	-0.132420
H	2.041709	1.262223	-1.496281
H	2.190085	0.679579	1.528744
O	1.737614	-0.863806	0.187312
O	-0.511666	-0.775005	1.461593
O	-0.302812	-1.636336	-1.100654
O	-1.917283	0.042326	-0.448074
C	-2.527292	1.078181	0.304827
H	-2.014350	2.041483	0.169087
H	-2.543809	0.844684	1.378901
H	3.436047	0.355493	0.271658
H	-3.563154	1.187569	-0.041673

Native Intermediate Structure at the PCM-B3LYP/6-311+G(d,p) level:

No intermediate could be determined by us that satisfies all default criteria in GAUSSIAN 09.

Native Late Transition State (LTS) Structure at the PCM-B3LYP/6-311+G(d,p) level:

P	-0.003031	-0.613064	-0.005694
O	0.170402	1.017041	-0.365118
C	1.538449	1.479992	-0.444412
C	2.338259	0.521510	0.423363
H	1.566234	2.526720	-0.088213
H	1.870730	1.433936	-1.501916
H	2.237625	0.784117	1.500171
O	1.753363	-0.750685	0.156137
O	-0.432768	-0.917985	1.425568
O	-0.185189	-1.592511	-1.158035
O	-2.172395	-0.002054	-0.469353
C	-2.757579	0.998768	0.302405
H	-2.340217	2.007756	0.101070
H	-2.632528	0.830634	1.392822
H	3.411173	0.504822	0.152519
H	-3.849629	1.075910	0.127219

Native Dianionic Reactant Structure at the PCM-M06-2X/6-311+G(d,p) level:

C	-1.158605	2.148235	-0.085606
O	-1.345241	0.919297	-0.794628
P	-1.186101	-0.484918	0.028452
O	-1.269954	-1.565932	-1.009774
O	0.316198	-0.369657	0.628898
C	1.441348	-0.313405	-0.275934
C	2.690589	0.081591	0.510679
O	3.809757	0.112313	-0.301940
O	-2.107469	-0.492188	1.214938
H	1.578893	-1.307749	-0.744595
H	1.239254	0.435929	-1.069782
H	2.466776	1.068460	0.990836
H	2.779554	-0.649443	1.354227
H	-1.349892	2.958448	-0.792752
H	-1.859807	2.219191	0.753901
H	-0.129582	2.219737	0.286613

Native Early Transition State (ETS) Structure at the PCM-M06-2X/6-311+G(d,p) level:

P	-0.344517	-0.514009	-0.048587
O	0.236944	0.973328	-0.477633
C	1.624108	1.321030	-0.506671
C	2.347341	0.409703	0.469498
H	1.696836	2.395919	-0.255049
H	2.003014	1.153711	-1.535192
H	2.127589	0.754937	1.511612
O	1.860314	-0.861306	0.222542
O	-0.487612	-0.753832	1.447112
O	-0.286705	-1.623984	-1.082370
O	-1.932022	0.019379	-0.429385
C	-2.507165	1.071532	0.321324
H	-1.973772	2.016549	0.157203
H	-2.500232	0.843979	1.394477
H	3.446014	0.510762	0.316070
H	-3.544756	1.191994	-0.007345

Native Intermediate Structure at the PCM-M06-2X/6-311+G(d,p) level:

P	-0.232286	-0.534264	-0.029104
O	0.260350	0.989349	-0.571958
C	1.633651	1.355692	-0.467866
C	2.257031	0.344972	0.483854
H	1.694749	2.398970	-0.105111
H	2.099320	1.284656	-1.471302
H	2.052518	0.635873	1.539840
O	1.622327	-0.856156	0.152115
O	-0.481653	-0.656430	1.480991
O	-0.344597	-1.707967	-1.009731
O	-1.880413	0.036594	-0.444117
C	-2.441181	1.099219	0.287833
H	-1.866684	2.028521	0.167561
H	-2.493838	0.866882	1.360019
H	3.353377	0.280273	0.342277
H	-3.460262	1.276364	-0.078047

Native Late Transition State (LTS) Structure at the PCM-M06-2X/6-311+G(d,p) level:

P	0.042874	-0.631937	0.004466
O	0.130329	0.964465	-0.431773
C	1.464430	1.495626	-0.465668
C	2.281626	0.569560	0.420569
H	1.435024	2.538711	-0.102279
H	1.833345	1.466301	-1.510303
H	2.122501	0.807508	1.494779
O	1.761280	-0.715104	0.115524
O	-0.367373	-0.852868	1.443176
O	-0.185247	-1.643010	-1.093453
O	-2.235036	-0.078134	-0.413724
C	-2.697552	1.027041	0.280060
H	-2.304384	1.984458	-0.116575
H	-2.411792	1.007019	1.351956
H	3.361217	0.602245	0.188045
H	-3.801688	1.116662	0.259622

Native Dianionic Reactant Structure at the PCM-MP2/6-311+G(d,p) level:

C	-1.121953	2.168770	-0.102172
O	-1.290525	0.932807	-0.816348
P	-1.191581	-0.475123	0.028783
O	-1.304387	-1.562757	-1.009726
O	0.312693	-0.417943	0.658167
C	1.453051	-0.432395	-0.239301
C	2.664926	0.133307	0.499593
O	3.799479	0.118210	-0.310611
O	-2.130569	-0.439919	1.209742
H	1.647343	-1.475776	-0.557982
H	1.233331	0.188373	-1.132069
H	2.381959	1.162729	0.836331
H	2.783763	-0.474582	1.432512
H	-1.210883	2.970972	-0.840105
H	-1.899474	2.283636	0.662706
H	-0.131994	2.210227	0.368358

Native Early Transition State (ETS) Structure at the PCM-MP2/6-311+G(d,p) level:

P	-0.311874	-0.519199	-0.042878
O	0.246845	0.993904	-0.491069
C	1.642230	1.323544	-0.501956
C	2.329199	0.395806	0.482094
H	1.727571	2.397139	-0.241522
H	2.036582	1.149759	-1.524322
H	2.101031	0.739484	1.521990
O	1.794856	-0.864862	0.215619
O	-0.506742	-0.736767	1.459717
O	-0.291754	-1.644265	-1.076389
O	-1.917171	0.037693	-0.458497
C	-2.504807	1.069490	0.319139
H	-1.910099	1.992563	0.284012
H	-2.618606	0.767610	1.368964
H	3.432000	0.445460	0.339608
H	-3.498383	1.277304	-0.096264

Native Intermediate Structure at the PCM-MP2/6-311+G(d,p) level:

P	-0.236914	-0.534971	-0.028581
O	0.263192	0.999717	-0.565067
C	1.648533	1.348348	-0.476882
C	2.265275	0.354032	0.491827
H	1.720412	2.400256	-0.136537
H	2.108328	1.244666	-1.481279
H	2.040397	0.658864	1.540429
O	1.641529	-0.861363	0.163071
O	-0.497518	-0.660653	1.484485
O	-0.338884	-1.710935	-1.016407
O	-1.883788	0.049550	-0.468174
C	-2.458881	1.091678	0.296277
H	-1.823949	1.989285	0.313751
H	-2.639639	0.782140	1.335580
H	3.364903	0.294519	0.363253
H	-3.422547	1.359969	-0.157074

Native Late Transition State (LTS) Structure at the PCM-MP2/6-311+G(d,p) level:

P	0.010413	-0.617021	0.000548
O	0.163859	0.992896	-0.416981
C	1.527260	1.451647	-0.487773
C	2.294431	0.541511	0.451424
H	1.546174	2.517071	-0.189688
H	1.893610	1.334199	-1.528486
H	2.111562	0.832246	1.509506
O	1.744715	-0.743748	0.180694
O	-0.455053	-0.848885	1.427918
O	-0.176251	-1.627312	-1.116908
O	-2.176356	0.005003	-0.507951
C	-2.704773	0.994289	0.319491
H	-2.257240	1.993075	0.139242
H	-2.542315	0.778456	1.394231
H	3.381334	0.533979	0.243939
H	-3.798140	1.117968	0.190010

S3′ Dianionic Reactant Structure at the Gas-HF/3-21+G* level:

C	1.707824	2.175619	-0.047191
O	1.490064	1.007941	0.769506
P	1.387876	-0.506833	0.145350
O	1.317632	-1.438723	1.307985
S	-0.416482	-0.437672	-0.932829
C	-1.736661	-0.142608	0.328270
C	-3.114076	0.116807	-0.356344
O	-4.140066	0.354833	0.583676
O	2.456348	-0.625680	-0.905159
H	-1.809837	-1.004224	0.974199
H	-1.470055	0.716959	0.925908
H	-2.968143	0.962248	-1.046762
H	-3.319029	-0.756482	-0.995325
H	1.839290	3.005447	0.635100
H	2.590005	2.043578	-0.660805
H	0.848999	2.351846	-0.683788

S3′ Early Transition State (ETS) Structure at the Gas-HF/3-21+G* level:

P	-0.554600	-0.618511	-0.150789
S	0.448008	1.285324	-0.504523
C	2.211582	1.092614	-0.087085
C	2.407494	-0.202090	0.742231
H	2.536121	1.984967	0.447906
H	2.781621	0.998582	-1.004907
H	2.011033	-0.028995	1.750951
O	1.758879	-1.244151	0.075023
O	-0.701698	-0.960707	1.308579
O	-0.625405	-1.562077	-1.307528
O	-2.001315	0.277868	-0.397531
C	-2.697095	0.909480	0.681360
H	-2.065865	1.631459	1.191919
H	-3.030980	0.176739	1.406681
H	3.497026	-0.361102	0.845109
H	-3.553666	1.423339	0.249149

S3′ Intermediate Structure at the Gas-HF/3-21+G* level:

No intermediate could be determined by us that satisfies all default criteria in GAUSSIAN 09.

S3′ Late Transition State (LTS) Structure at the Gas-HF/3-21+G* level:

P	-0.093478	-0.791655	-0.107325
S	0.247767	1.327099	-0.371277
C	2.070118	1.292286	-0.081589
C	2.352693	-0.011924	0.681317
H	2.368535	2.164024	0.495839
H	2.616955	1.287505	-1.019971
H	2.034079	0.081261	1.716109
O	1.605940	-1.034895	0.017103
O	-0.556278	-1.116301	1.288402
O	-0.399923	-1.614748	-1.318050
O	-2.077875	0.464345	-0.463490
C	-3.026251	0.660203	0.558692
H	-3.073342	1.712539	0.903563
H	-2.812313	0.048433	1.439979
H	3.401736	-0.291501	0.646703
H	-4.052024	0.408362	0.225847

S3′ Dianionic Reactant Structure at the Gas-B3LYP/6-31+G(d) level:

C	1.760229	2.123551	-0.021027
O	1.533190	1.020969	0.834921
P	1.416405	-0.516834	0.131958
O	1.339876	-1.462574	1.303976
S	-0.449538	-0.400961	-0.957833
C	-1.798743	-0.177567	0.325172
C	-3.175808	0.194667	-0.320720
O	-4.168559	0.301386	0.589362
O	2.484170	-0.610296	-0.943429
H	-1.899536	-1.110299	0.888884
H	-1.492035	0.614801	1.015951
H	-2.981758	1.139405	-0.912204
H	-3.357112	-0.591329	-1.116356
H	1.806831	3.022320	0.611541
H	2.704890	2.013640	-0.573737
H	0.941768	2.239561	-0.747307

S3′ Early Transition State (ETS) Structure at the Gas-B3LYP/6-31+G(d) level:

P	-0.533915	-0.652053	-0.143051
S	0.482934	1.379386	-0.478171
C	2.240458	1.065560	-0.040675
C	2.340674	-0.297887	0.700315
H	2.615411	1.895857	0.583905
H	2.838886	1.016510	-0.963281
H	1.972297	-0.132535	1.749598
O	1.669945	-1.259272	0.036120
O	-0.726569	-1.022773	1.320966
O	-0.647439	-1.550193	-1.355283
O	-2.036420	0.308693	-0.420101
C	-2.624570	0.940445	0.679943
H	-1.936122	1.640930	1.186441
H	-2.975055	0.220067	1.439977
H	3.445919	-0.512353	0.794263
H	-3.495060	1.521811	0.314483

S3′ Intermediate Structure at the Gas-B3LYP/6-31+G(d) level:

P	-0.479907	-0.501167	-0.053143
S	0.859356	1.506246	-0.109175
C	2.501228	0.693718	-0.062120
C	2.250384	-0.770412	0.359384
H	3.170899	1.202272	0.652039
H	2.978463	0.709360	-1.055887
H	2.046521	-0.800385	1.451243
O	1.207929	-1.296230	-0.374660
O	-0.664593	-1.050934	1.365740
O	-1.084211	-1.114927	-1.316493
O	-1.702556	0.916109	0.081246
C	-3.033848	0.531930	0.157581
H	-3.237512	-0.123220	1.030203
H	-3.373828	-0.008816	-0.748356
H	3.170171	-1.366444	0.170147
H	-3.664952	1.441230	0.268822

S3′ Late Transition State (LTS) Structure at the Gas-B3LYP/6-31+G(d) level:

P	-0.156564	-0.805646	-0.098340
S	0.271024	1.376692	-0.410332
C	2.092442	1.281173	-0.066415
C	2.315707	-0.051727	0.669112
H	2.411496	2.137932	0.549297
H	2.672979	1.287258	-1.003029
H	1.967496	0.048315	1.716788
O	1.635250	-1.065758	-0.000855
O	-0.567015	-1.117538	1.331537
O	-0.433083	-1.654306	-1.317524
O	-2.143192	0.378666	-0.487790
C	-2.894070	0.756011	0.581202
H	-2.945618	1.876919	0.735269
H	-2.529070	0.333926	1.545109
H	3.393849	-0.306437	0.690441
H	-3.979203	0.438444	0.500201

S3′ Dianionic Reactant Structure at the Gas-M06-2X/6-31+G(d) level:

C	1.622584	2.116371	-0.042465
O	1.437554	1.028387	0.828850
P	1.407366	-0.495648	0.140851
O	1.338094	-1.443160	1.298238
S	-0.425553	-0.443685	-0.961999
C	-1.724973	-0.170329	0.323060
C	-3.110524	0.144220	-0.320197
O	-4.089520	0.304845	0.585539
O	2.489828	-0.539183	-0.907580
H	-1.804222	-1.066694	0.945368
H	-1.419121	0.667799	0.958395
H	-2.925464	1.044245	-0.977243
H	-3.286833	-0.694541	-1.057684
H	1.621567	3.028644	0.567596
H	2.575119	2.031504	-0.582454
H	0.807155	2.174042	-0.777528

S3′ Early Transition State (ETS) Structure at the Gas-M06-2X/6-31+G(d) level:

P	-0.571969	-0.636258	-0.144048
S	0.436078	1.318503	-0.549303
C	2.177817	1.098148	-0.050027
C	2.336126	-0.237787	0.723779
H	2.485413	1.965476	0.557288
H	2.799729	1.052717	-0.954699
H	1.879453	-0.076560	1.738435
O	1.799593	-1.251131	0.042117
O	-0.656884	-0.961550	1.325115
O	-0.642408	-1.571194	-1.312049
O	-2.062605	0.245012	-0.387823
C	-2.572171	0.932209	0.714168
H	-1.830853	1.620397	1.150751
H	-2.895385	0.245201	1.511391
H	3.451738	-0.327619	0.906695
H	-3.440017	1.523686	0.373316

S3′ Intermediate Structure at the Gas-M06-2X/6-31+G(d) level:

P	-0.476919	-0.478075	-0.056966
S	0.876958	1.482607	-0.123007
C	2.490802	0.647883	-0.043990
C	2.182552	-0.805081	0.357813
H	3.154863	1.129571	0.690003
H	2.992498	0.653478	-1.023903
H	1.939265	-0.838347	1.438084
O	1.138856	-1.271696	-0.406916
O	-0.635779	-1.015696	1.360849
O	-1.123528	-1.069541	-1.299691
O	-1.651362	0.922173	0.104264
C	-2.973243	0.519181	0.167871
H	-3.138022	-0.229625	0.965620
H	-3.322189	0.076296	-0.782688
H	3.076886	-1.436388	0.182506
H	-3.607012	1.400620	0.394770

S3′ Late Transition State (LTS) Structure at the Gas-M06-2X/6-31+G(d) level:

P	-0.029826	-0.857622	-0.076835
S	0.120969	1.304717	-0.464110
C	1.926920	1.410598	-0.106337
C	2.276020	0.142737	0.679011
H	2.150787	2.315436	0.476652
H	2.517251	1.434904	-1.034089
H	1.882395	0.227407	1.708129
O	1.716802	-0.948691	0.020434
O	-0.455522	-1.123853	1.342002
O	-0.290917	-1.732459	-1.262631
O	-2.237638	0.255455	-0.498068
C	-2.869357	0.733142	0.594622
H	-2.832425	1.859833	0.701658
H	-2.461096	0.336218	1.555106
H	3.368884	-0.004834	0.731275
H	-3.977203	0.497428	0.621879

S3′ Dianionic Reactant Structure at the Gas-B3LYP/6-311+G(d,p) level:

C	1.740302	2.130309	-0.032122
O	1.528252	1.025574	0.823727
P	1.422361	-0.514870	0.134298
O	1.360388	-1.451809	1.306048
S	-0.454278	-0.417210	-0.954855
C	-1.797291	-0.170210	0.329559
C	-3.177008	0.182878	-0.318038
O	-4.164889	0.304670	0.590093
O	2.485520	-0.602669	-0.937989
H	-1.890489	-1.090057	0.909317
H	-1.487263	0.635950	0.997511
H	-2.986310	1.111909	-0.931447
H	-3.354574	-0.617545	-1.096945
H	1.797342	3.026663	0.597684
H	2.672512	2.021010	-0.601125
H	0.911624	2.246498	-0.743210

S3′ Early Transition State (ETS) Structure at the Gas-B3LYP/6-311+G(d,p) level:

P	-0.530119	-0.660215	-0.142470
S	0.491587	1.385193	-0.483173
C	2.241897	1.060436	-0.034737
C	2.327377	-0.303838	0.701734
H	2.613080	1.884346	0.594330
H	2.841636	1.010438	-0.952896
H	1.952441	-0.138391	1.745691
O	1.653295	-1.257713	0.032270
O	-0.725034	-1.021378	1.317819
O	-0.652434	-1.552378	-1.349459
O	-2.036324	0.307140	-0.415462
C	-2.617337	0.954993	0.677249
H	-1.952147	1.715501	1.121806
H	-2.889966	0.253718	1.481565
H	3.425668	-0.529177	0.803047
H	-3.531971	1.468783	0.327466

S3′ Intermediate Structure at the Gas-B3LYP/6-311+G(d,p) level:

P	-0.471188	-0.504623	-0.053174
S	0.836058	1.502996	-0.102802
C	2.488911	0.716038	-0.068674
C	2.270660	-0.749153	0.359581
H	3.150024	1.241824	0.635680
H	2.948905	0.737453	-1.066852
H	2.072536	-0.774918	1.451174
O	1.238467	-1.298278	-0.365064
O	-0.656975	-1.059624	1.355364
O	-1.059390	-1.105862	-1.320741
O	-1.724105	0.905359	0.087663
C	-3.049727	0.512196	0.153042
H	-3.257041	-0.141254	1.024432
H	-3.375838	-0.037436	-0.750728
H	3.203100	-1.321921	0.173871
H	-3.693845	1.410412	0.253406

S3′ Late Transition State (LTS) Structure at the Gas-B3LYP/6-311+G(d,p) level:

P	-0.169806	-0.800243	-0.105564
S	0.298919	1.389153	-0.400932
C	2.114719	1.255457	-0.061344
C	2.314164	-0.077624	0.675427
H	2.447521	2.105370	0.550529
H	2.686564	1.246800	-0.999549
H	1.962228	0.031501	1.718795
O	1.623006	-1.081641	0.006597
O	-0.587676	-1.115616	1.314623
O	-0.442762	-1.631001	-1.329114
O	-2.135791	0.403065	-0.483134
C	-2.906416	0.746967	0.581358
H	-2.944387	1.858047	0.784078
H	-2.571887	0.280583	1.533002
H	3.386420	-0.344501	0.703943
H	-3.991082	0.452131	0.463145

S3′ Dianionic Reactant Structure at the Gas-M06-2X/6-311+G(d,p) level:

C	1.350685	2.173350	-0.089549
O	1.334139	1.083284	0.800173
P	1.443746	-0.447947	0.148992
O	1.469614	-1.369957	1.321469
S	-0.396854	-0.581047	-0.947563
C	-1.702639	-0.298030	0.331245
C	-3.044369	0.167241	-0.312362
O	-4.044313	0.277614	0.574901
O	2.520894	-0.418684	-0.897975
H	-1.866779	-1.227708	0.878136
H	-1.340629	0.459926	1.029275
H	-2.783672	1.119879	-0.853648
H	-3.236564	-0.567204	-1.146483
H	1.358548	3.087796	0.511711
H	2.239368	2.141729	-0.730308
H	0.458469	2.168104	-0.727094

S3′ Early Transition State (ETS) Structure at the Gas-M06-2X/6-311+G(d,p) level:

P	-0.573376	-0.640001	-0.144400
S	0.437473	1.317488	-0.560821
C	2.174737	1.100970	-0.044072
C	2.329934	-0.235166	0.728932
H	2.467457	1.967492	0.565334
H	2.798112	1.057366	-0.944012
H	1.853761	-0.079029	1.731125
O	1.809162	-1.249292	0.037752
O	-0.646390	-0.958284	1.321698
O	-0.647442	-1.574639	-1.304024
O	-2.066456	0.236427	-0.378181
C	-2.570886	0.940276	0.716187
H	-1.841124	1.662088	1.110267
H	-2.846459	0.268290	1.539848
H	3.439002	-0.318686	0.928334
H	-3.463385	1.492495	0.384004

S3′ Intermediate Structure at the Gas-M06-2X/6-311+G(d,p) level:

P	-0.471716	-0.479876	-0.061141
S	0.866498	1.480839	-0.121193
C	2.485894	0.657736	-0.044141
C	2.190966	-0.794313	0.366018
H	3.141706	1.150977	0.684310
H	2.976212	0.663586	-1.026039
H	1.941604	-0.820158	1.442505
O	1.154128	-1.273622	-0.398375
O	-0.636721	-1.020712	1.348636
O	-1.106300	-1.061078	-1.307169
O	-1.663306	0.917138	0.103257
C	-2.982220	0.508269	0.174889
H	-3.137499	-0.234299	0.977477
H	-3.328302	0.053208	-0.768642
H	3.090156	-1.415444	0.200250
H	-3.622349	1.382889	0.394938

S3′ Late Transition State (LTS) Structure at the Gas-M06-2X/6-311+G(d,p) level:

P	-0.024840	-0.862557	-0.080579
S	0.119409	1.307267	-0.461998
C	1.925607	1.411291	-0.110190
C	2.273360	0.152959	0.687430
H	2.147646	2.319922	0.460977
H	2.505868	1.420442	-1.040712
H	1.871663	0.246378	1.709833
O	1.719239	-0.945427	0.036731
O	-0.462359	-1.134855	1.327491
O	-0.273639	-1.727977	-1.267874
O	-2.242120	0.259461	-0.498313
C	-2.876878	0.727577	0.597693
H	-2.815765	1.847215	0.729038
H	-2.486204	0.304148	1.551016
H	3.362849	0.008899	0.747193
H	-3.985501	0.514507	0.609409

S3′ Dianionic Reactant Structure at the Gas-MP2/6-311+G(d,p) level:

C	1.405371	2.169701	-0.108673
O	1.314391	1.091338	0.800646
P	1.438641	-0.450653	0.149252
O	1.491599	-1.369829	1.333328
S	-0.412955	-0.612279	-0.929494
C	-1.706706	-0.283320	0.335851
C	-3.046452	0.163955	-0.321373
O	-4.050262	0.320117	0.570549
O	2.508529	-0.408597	-0.915467
H	-1.886342	-1.189786	0.920598
H	-1.352743	0.504537	1.006946
H	-2.781884	1.093681	-0.900241
H	-3.249137	-0.604735	-1.123078
H	1.243474	3.090648	0.463197
H	2.389677	2.201198	-0.592254
H	0.637283	2.094465	-0.889314

S3′ Early Transition State (ETS) Structure at the Gas-MP2/6-311+G(d,p) level:

P	-0.547976	-0.648078	-0.144221
S	0.451435	1.334810	-0.541104
C	2.180852	1.085911	-0.048304
C	2.306339	-0.246955	0.730941
H	2.510902	1.940650	0.565014
H	2.808654	1.013229	-0.946628
H	1.841408	-0.072792	1.736791
O	1.741091	-1.254265	0.044293
O	-0.667502	-0.967962	1.327074
O	-0.637936	-1.569545	-1.324770
O	-2.049507	0.266854	-0.402867
C	-2.569500	0.937648	0.711137
H	-1.836708	1.621563	1.167121
H	-2.899575	0.242232	1.497489
H	3.412147	-0.373829	0.914475
H	-3.435453	1.532873	0.374218

S3′ Intermediate Structure at the Gas-MP2/6-311+G(d,p) level:

P	-0.462472	-0.490270	-0.050086
S	0.834108	1.482039	-0.113395
C	2.466389	0.698295	-0.062827
C	2.222347	-0.759627	0.357401
H	3.126287	1.206943	0.656358
H	2.943820	0.701678	-1.053775
H	1.977141	-0.780832	1.437350
O	1.200282	-1.282554	-0.406790
O	-0.609811	-1.045136	1.362576
O	-1.091795	-1.071974	-1.305755
O	-1.684981	0.911285	0.126952
C	-3.009253	0.495501	0.145797
H	-3.194642	-0.279943	0.912985
H	-3.338606	0.080407	-0.824033
H	3.146165	-1.347620	0.192783
H	-3.655263	1.362817	0.385866

S3′ Late Transition State (LTS) Structure at the Gas-MP2/6-311+G(d,p) level:

P	-0.102527	-0.834280	-0.087359
S	0.197866	1.330762	-0.459913
C	1.992122	1.340133	-0.095974
C	2.266834	0.057728	0.694303
H	2.262184	2.230358	0.490400
H	2.588794	1.319334	-1.019190
H	1.853047	0.167831	1.712973
O	1.675848	-1.010642	0.022901
O	-0.511093	-1.100820	1.340745
O	-0.360057	-1.698942	-1.284758
O	-2.177887	0.291087	-0.491992
C	-2.841910	0.768732	0.595730
H	-2.764459	1.886321	0.732421
H	-2.483749	0.331785	1.554836
H	3.351415	-0.130631	0.768852
H	-3.951953	0.571994	0.569187

S3′ Dianionic Reactant Structure at the PCM-HF/3-21+G* level:

C	1.881679	2.166815	-0.114498
O	1.542482	0.992530	0.706481
P	1.322246	-0.506414	0.166029
O	1.134428	-1.362798	1.388783
S	-0.423188	-0.428165	-0.963193
C	-1.694052	0.016109	0.290752
C	-3.090048	0.075954	-0.367819
O	-4.093488	0.406394	0.610812
O	2.412643	-0.862120	-0.811319
H	-1.692082	-0.733025	1.075423
H	-1.446249	0.983013	0.717750
H	-3.061807	0.819606	-1.174212
H	-3.294525	-0.897201	-0.831804
H	2.017159	2.980487	0.582333
H	2.794791	1.972021	-0.662037
H	1.066041	2.376633	-0.795455

S3′ Early Transition State (ETS) Structure at the PCM-HF/3-21+G* level:

P	-0.520071	-0.573536	-0.132024
S	0.427427	1.299703	-0.418817
C	2.214331	1.103005	-0.098035
C	2.441479	-0.199011	0.683636
H	2.548767	1.979201	0.452330
H	2.733127	1.059700	-1.050911
H	2.126280	-0.056760	1.725244
O	1.675902	-1.222863	0.042995
O	-0.679299	-1.044912	1.304932
O	-0.560183	-1.549228	-1.295473
O	-1.988731	0.197920	-0.399640
C	-2.764830	0.916872	0.604114
H	-2.164589	1.689332	1.071998
H	-3.122959	0.227376	1.357849
H	3.513298	-0.429140	0.682927
H	-3.599091	1.365553	0.081183

S3′ Intermediate Structure at the PCM-HF/3-21+G* level:

P	-0.382069	-0.622876	-0.123651
S	0.490790	1.342677	-0.433067
C	2.240039	1.022950	-0.046218
C	2.257665	-0.317836	0.704279
H	2.635144	1.829049	0.565505
H	2.817075	0.953432	-0.963524
H	1.960215	-0.174982	1.747145
O	1.319707	-1.181582	0.025069
O	-0.762328	-1.042802	1.308997
O	-0.634300	-1.550281	-1.327247
O	-1.882516	0.288288	-0.420079
C	-2.612022	1.014181	0.597646
H	-1.953175	1.650291	1.180923
H	-3.116642	0.326437	1.267198
H	3.244416	-0.780477	0.666061
H	-3.347232	1.631795	0.092378

S3′ Late Transition State (LTS) Structure at the PCM-HF/3-21+G* level:

P	-0.089599	-0.766973	-0.071062
S	0.211152	1.298707	-0.382281
C	2.026519	1.321635	-0.144535
C	2.381399	0.048444	0.631948
H	2.304514	2.212496	0.411894
H	2.524308	1.330283	-1.109411
H	2.135852	0.151951	1.691777
O	1.574443	-1.020210	0.045669
O	-0.554585	-1.178180	1.316958
O	-0.395397	-1.639657	-1.274972
O	-2.161666	0.109163	-0.428345
C	-2.885580	0.912116	0.521286
H	-2.832913	1.974802	0.272993
H	-2.488024	0.791391	1.530575
H	3.426947	-0.230273	0.511043
H	-3.941502	0.632541	0.546887

S3′ Dianionic Reactant Structure at the PCM-B3LYP/6-31+G(d) level:

C	1.994962	2.074460	-0.069179
O	1.599315	0.983050	0.785054
P	1.337611	-0.523457	0.150985
O	1.118576	-1.406254	1.366055
S	-0.458354	-0.338292	-0.990899
C	-1.748870	0.008297	0.306187
C	-3.147861	0.128331	-0.340891
O	-4.132054	0.362912	0.612748
O	2.418897	-0.856462	-0.864190
H	-1.738247	-0.816865	1.033105
H	-1.485929	0.945556	0.819714
H	-3.087975	0.944702	-1.109140
H	-3.324618	-0.817942	-0.918847
H	2.085151	2.955209	0.576169
H	2.960500	1.862116	-0.545894
H	1.233357	2.259266	-0.839520

S3′ Early Transition State (ETS) Structure at the PCM-B3LYP/6-31+G(d) level:

P	-0.519276	-0.596474	-0.125775
S	0.441306	1.360881	-0.402747
C	2.235441	1.085068	-0.086341
C	2.411671	-0.248504	0.658239
H	2.608299	1.942116	0.497888
H	2.756533	1.055246	-1.055804
H	2.097265	-0.098344	1.725069
O	1.682601	-1.246978	0.030535
O	-0.708336	-1.074036	1.319953
O	-0.586622	-1.542765	-1.330405
O	-2.037088	0.215134	-0.426913
C	-2.706413	0.925911	0.613180
H	-2.061100	1.693640	1.066207
H	-3.052797	0.245816	1.404541
H	3.507472	-0.472413	0.676803
H	-3.576061	1.421266	0.160049

S3′ Intermediate Structure at the PCM-B3LYP/6-31+G(d) level:

P	-0.402608	-0.642199	-0.118636
S	0.495837	1.388912	-0.423475
C	2.255333	1.024771	-0.039519
C	2.255574	-0.328653	0.683323
H	2.669021	1.826304	0.592036
H	2.833026	0.969575	-0.975291
H	1.942979	-0.183666	1.744649
O	1.390357	-1.212968	0.009683
O	-0.767169	-1.077471	1.321369
O	-0.638642	-1.550271	-1.349472
O	-1.962043	0.295809	-0.438528
C	-2.590418	1.013366	0.607800
H	-1.890107	1.679073	1.138869
H	-3.047738	0.340868	1.352046
H	3.281081	-0.755351	0.681150
H	-3.385502	1.635903	0.167646

S3′ Late Transition State (LTS) Structure at the PCM-B3LYP/6-31+G(d) level:

P	-0.135581	-0.765485	-0.074206
S	0.258472	1.354894	-0.378497
C	2.086854	1.277442	-0.125601
C	2.354005	-0.024186	0.632048
H	2.411779	2.157445	0.450651
H	2.594203	1.275169	-1.102543
H	2.078148	0.090520	1.704377
O	1.591010	-1.065835	0.025562
O	-0.588773	-1.173014	1.332308
O	-0.429293	-1.631143	-1.302528
O	-2.208131	0.151698	-0.455564
C	-2.842458	0.904170	0.534304
H	-2.656204	1.996924	0.440387
H	-2.516083	0.619053	1.556130
H	3.423497	-0.308086	0.565730
H	-3.946099	0.774726	0.511567

S3′ Dianionic Reactant Structure at the PCM-M06-2X/6-31+G(d) level:

C	1.824892	2.087725	-0.075782
O	1.502901	0.996714	0.790950
P	1.335268	-0.504942	0.156518
O	1.126150	-1.401507	1.350169
S	-0.431311	-0.379367	-0.999849
C	-1.683859	-0.025470	0.298161
C	-3.080735	0.107616	-0.337605
O	-4.052794	0.346900	0.613008
O	2.443887	-0.772221	-0.832073
H	-1.679490	-0.849544	1.026683
H	-1.411135	0.910492	0.809957
H	-3.010752	0.922507	-1.104811
H	-3.261521	-0.835519	-0.917161
H	1.873273	2.983644	0.550399
H	2.793726	1.919817	-0.561497
H	1.044923	2.214293	-0.838832

S3′ Early Transition State (ETS) Structure at the PCM-M06-2X/6-31+G(d) level:

P	-0.550156	-0.586538	-0.130072
S	0.419096	1.322688	-0.448280
C	2.196651	1.096463	-0.085295
C	2.394276	-0.216446	0.680047
H	2.531170	1.973030	0.490584
H	2.740485	1.060984	-1.040931
H	2.008727	-0.065208	1.722795
O	1.751606	-1.243753	0.029275
O	-0.674470	-1.031001	1.318069
O	-0.578755	-1.552791	-1.300841
O	-2.041370	0.188764	-0.412132
C	-2.657208	0.919487	0.637510
H	-1.961509	1.640614	1.088950
H	-3.026568	0.245773	1.421317
H	3.497715	-0.373521	0.770406
H	-3.501616	1.466614	0.201904

S3′ Intermediate Structure at the PCM-M06-2X/6-31+G(d) level:

P	-0.404888	-0.635549	-0.121686
S	0.506387	1.365582	-0.458521
C	2.236310	0.994540	-0.029677
C	2.189150	-0.347323	0.704379
H	2.645779	1.793403	0.605338
H	2.840316	0.914564	-0.945466
H	1.833351	-0.186925	1.748281
O	1.333838	-1.207634	0.004696
O	-0.761557	-1.023889	1.324395
O	-0.660088	-1.550096	-1.332397
O	-1.925326	0.299106	-0.431689
C	-2.500002	1.033894	0.621034
H	-1.749093	1.615725	1.177971
H	-3.017422	0.379161	1.338817
H	3.202696	-0.794947	0.745242
H	-3.232173	1.736384	0.196977

S3′ Late Transition State (LTS) Structure at the PCM-M06-2X/6-31+G(d) level:

P	-0.064347	-0.794345	-0.064183
S	0.183386	1.313288	-0.416076
C	1.995459	1.336149	-0.143609
C	2.322556	0.067884	0.638785
H	2.268635	2.239163	0.420851
H	2.516415	1.338921	-1.112045
H	2.013476	0.178233	1.701521
O	1.626840	-1.010519	0.030967
O	-0.533619	-1.155401	1.334159
O	-0.372597	-1.668657	-1.264357
O	-2.274120	0.087105	-0.447575
C	-2.796858	0.901061	0.542976
H	-2.688333	1.985546	0.322794
H	-2.301518	0.739351	1.523523
H	3.404714	-0.160114	0.595832
H	-3.881349	0.730676	0.713022

S3′ Dianionic Reactant Structure at the PCM-B3LYP/6-311+G(d,p) level:

C	2.001330	2.074868	-0.073277
O	1.597302	0.982400	0.775628
P	1.337200	-0.524618	0.153024
O	1.119997	-1.398716	1.367354
S	-0.463516	-0.344865	-0.993806
C	-1.748870	0.013910	0.304641
C	-3.148105	0.128847	-0.337578
O	-4.127931	0.366801	0.617113
O	2.417535	-0.858617	-0.854316
H	-1.733608	-0.805414	1.034212
H	-1.480489	0.953389	0.805531
H	-3.090142	0.938824	-1.111479
H	-3.323490	-0.819317	-0.911246
H	2.087585	2.954229	0.570497
H	2.968523	1.862871	-0.542068
H	1.248521	2.261829	-0.848864

S3′ Early Transition State (ETS) Structure at the PCM-B3LYP/6-311+G(d,p) level:

P	-0.517897	-0.601586	-0.125929
S	0.445289	1.365623	-0.399440
C	2.237341	1.080192	-0.088180
C	2.407636	-0.250438	0.657995
H	2.612220	1.935764	0.492008
H	2.751262	1.045092	-1.058335
H	2.095581	-0.095544	1.723693
O	1.674159	-1.245253	0.032500
O	-0.710146	-1.075022	1.314823
O	-0.585407	-1.540710	-1.328077
O	-2.035225	0.213771	-0.424700
C	-2.706741	0.930905	0.608947
H	-2.072552	1.717284	1.040377
H	-3.031511	0.261852	1.415740
H	3.501217	-0.479184	0.677538
H	-3.588864	1.402331	0.160021

S3′ Intermediate Structure at the PCM-B3LYP/6-311+G(d,p) level:

P	-0.403877	-0.647547	-0.118851
S	0.493093	1.392488	-0.418624
C	2.253431	1.026900	-0.045856
C	2.261141	-0.320640	0.682489
H	2.667454	1.831794	0.576559
H	2.818817	0.967010	-0.985751
H	1.948411	-0.170109	1.742125
O	1.402713	-1.212296	0.014316
O	-0.763474	-1.080749	1.315599
O	-0.630974	-1.548233	-1.347147
O	-1.969939	0.289159	-0.437004
C	-2.599602	1.011178	0.604737
H	-1.908155	1.699340	1.114172
H	-3.032267	0.345245	1.366056
H	3.289836	-0.737249	0.684807
H	-3.411858	1.609688	0.168439

S3′ Late Transition State (LTS) Structure at the PCM-B3LYP/6-311+G(d,p) level:

P	-0.148169	-0.763159	-0.077361
S	0.273891	1.363071	-0.372387
C	2.100179	1.258562	-0.127787
C	2.350320	-0.039636	0.635624
H	2.437016	2.136565	0.439630
H	2.597589	1.241061	-1.106747
H	2.071604	0.085471	1.705161
O	1.579073	-1.074788	0.032295
O	-0.602356	-1.169536	1.323249
O	-0.435535	-1.619309	-1.306455
O	-2.196768	0.159957	-0.456060
C	-2.838184	0.905743	0.534067
H	-2.643269	1.995695	0.457563
H	-2.529020	0.607360	1.554735
H	3.416760	-0.332390	0.576525
H	-3.939601	0.785880	0.496076

S3′ Dianionic Reactant Structure at the PCM-M06-2X/6-311+G(d,p) level:

C	1.809694	2.095150	-0.084728
O	1.488595	1.001945	0.780195
P	1.335789	-0.502918	0.159401
O	1.134902	-1.391667	1.353680
S	-0.432940	-0.398722	-1.002833
C	-1.679215	-0.027680	0.297445
C	-3.075564	0.109653	-0.336101
O	-4.044123	0.349672	0.617702
O	2.448800	-0.763774	-0.818317
H	-1.674200	-0.848439	1.026359
H	-1.393947	0.907701	0.798277
H	-3.003251	0.923607	-1.102014
H	-3.258318	-0.831265	-0.916190
H	1.842738	2.992460	0.537106
H	2.783723	1.935450	-0.559110
H	1.038575	2.211656	-0.855895

S3′ Early Transition State (ETS) Structure at the PCM-M06-2X/6-311+G(d,p) level:

P	-0.551086	-0.589448	-0.131310
S	0.420943	1.324517	-0.451766
C	2.197190	1.095210	-0.083668
C	2.389724	-0.215275	0.684490
H	2.526153	1.972075	0.490907
H	2.738921	1.056962	-1.037800
H	1.993302	-0.062798	1.721095
O	1.754184	-1.243259	0.028280
O	-0.669606	-1.031507	1.312737
O	-0.579183	-1.550933	-1.298556
O	-2.041847	0.185016	-0.406408
C	-2.659057	0.922245	0.638761
H	-1.969459	1.656872	1.072727
H	-3.011550	0.255944	1.433988
H	3.491459	-0.369344	0.785388
H	-3.513144	1.452123	0.205678

S3′ Intermediate Structure at the PCM-M06-2X/6-311+G(d,p) level:

P	-0.405296	-0.639365	-0.122514
S	0.505105	1.368867	-0.454643
C	2.235944	0.995155	-0.033948
C	2.191647	-0.341764	0.705996
H	2.646203	1.796726	0.593128
H	2.828994	0.909321	-0.953677
H	1.831567	-0.176423	1.746438
O	1.341180	-1.207179	0.008265
O	-0.758924	-1.027687	1.318568
O	-0.653452	-1.546472	-1.332347
O	-1.930087	0.294261	-0.430077
C	-2.507966	1.031845	0.619798
H	-1.762063	1.628039	1.163871
H	-3.009973	0.379064	1.346865
H	3.206992	-0.782605	0.752368
H	-3.251442	1.719701	0.196649

S3′ Late Transition State (LTS) Structure at the PCM-M06-2X/6-311+G(d,p) level:

P	-0.061945	-0.798139	-0.065266
S	0.182301	1.316786	-0.410600
C	1.996197	1.333377	-0.151156
C	2.321093	0.073363	0.641317
H	2.273161	2.240078	0.401275
H	2.505114	1.320996	-1.123441
H	2.004905	0.192277	1.700153
O	1.627292	-1.009208	0.038732
O	-0.534600	-1.159769	1.326086
O	-0.365859	-1.664435	-1.265080
O	-2.278065	0.083899	-0.448250
C	-2.799049	0.900634	0.542494
H	-2.684103	1.982213	0.324781
H	-2.307017	0.736032	1.521408
H	3.402860	-0.153085	0.605163
H	-3.882152	0.736852	0.711433

S3′ Dianionic Reactant Structure at the PCM-MP2/6-311+G(d,p) level:

C	1.761438	2.096111	-0.194658
O	1.429963	1.053172	0.736151
P	1.337483	-0.494037	0.189104
O	1.169355	-1.329838	1.434220
S	-0.430857	-0.498937	-0.983908
C	-1.643888	0.157981	0.219903
C	-3.077200	-0.082828	-0.282288
O	-4.019021	0.444131	0.595276
O	2.465624	-0.767638	-0.777612
H	-1.501521	-0.350696	1.184476
H	-1.471030	1.236268	0.348227
H	-3.141821	0.363238	-1.308894
H	-3.185734	-1.188518	-0.423613
H	1.671937	3.040726	0.348864
H	2.786097	1.973211	-0.562782
H	1.064074	2.093127	-1.042344

S3′ Early Transition State (ETS) Structure at the PCM-MP2/6-311+G(d,p) level:

P	-0.531470	-0.591161	-0.134559
S	0.432901	1.334014	-0.433592
C	2.199660	1.077534	-0.097188
C	2.374343	-0.221092	0.692839
H	2.565632	1.952485	0.463332
H	2.737002	1.000576	-1.053631
H	1.980948	-0.046345	1.727546
O	1.707885	-1.249491	0.047517
O	-0.692171	-1.037839	1.310411
O	-0.572173	-1.536951	-1.323787
O	-2.029393	0.212842	-0.427447
C	-2.659535	0.911093	0.643199
H	-1.970767	1.613945	1.130500
H	-3.043621	0.215860	1.399552
H	3.472477	-0.402918	0.786074
H	-3.496042	1.475886	0.215837

S3′ Intermediate Structure at the PCM-MP2/6-311+G(d,p) level:

P	-0.401877	-0.643195	-0.120460
S	0.496849	1.366026	-0.453166
C	2.226001	1.007232	-0.046292
C	2.197012	-0.317553	0.714056
H	2.642182	1.816837	0.571427
H	2.818607	0.900609	-0.966524
H	1.817691	-0.139332	1.746501
O	1.366929	-1.211561	0.015022
O	-0.757649	-1.030780	1.325628
O	-0.638498	-1.553815	-1.337281
O	-1.937906	0.294562	-0.441743
C	-2.523409	1.022936	0.620225
H	-1.782895	1.620686	1.171503
H	-3.027048	0.363094	1.341168
H	3.219397	-0.742827	0.775446
H	-3.269999	1.709494	0.197086

S3′ Late Transition State (LTS) Structure at the PCM-MP2/6-311+G(d,p) level:

P	-0.107650	-0.784682	-0.069407
S	0.210335	1.323653	-0.409771
C	2.013354	1.302671	-0.150152
C	2.302733	0.041341	0.653643
H	2.318099	2.205997	0.398804
H	2.533706	1.259516	-1.117868
H	1.960831	0.174005	1.704037
O	1.606996	-1.034823	0.035038
O	-0.556045	-1.153792	1.337066
O	-0.394085	-1.658242	-1.278778
O	-2.209086	0.110016	-0.449864
C	-2.768855	0.916880	0.542892
H	-2.700087	2.000022	0.313629
H	-2.268115	0.778375	1.520142
H	3.382911	-0.201440	0.642755
H	-3.843592	0.704675	0.709953

S5′ Dianionic Reactant Structure at the Gas-HF/3-21+G* level:

C	-1.699712	2.052817	0.531083
S	-1.701294	0.877036	-0.863292
P	-0.873600	-0.837073	0.130026
O	-0.841252	-1.889832	-0.933535
O	0.591537	-0.323783	0.502712
C	1.786020	-0.169058	-0.362656
C	2.968248	0.319598	0.487527
O	4.118809	0.500574	-0.319912
O	-1.646516	-1.013642	1.399286
H	2.002386	-1.125589	-0.814320
H	1.555266	0.553076	-1.134134
H	2.643888	1.245254	0.985165
H	3.116195	-0.418946	1.287631
H	-2.150178	2.982357	0.199153
H	-2.264501	1.641120	1.355483
H	-0.686308	2.239564	0.859174

S5′ Early Transition State (ETS) Structure at the Gas-HF/3-21+G* level:

P	0.016110	-0.623210	0.056983
O	0.455995	0.919662	-0.206261
C	1.765483	1.269955	-0.717180
C	2.788439	0.668916	0.255490
H	1.781265	2.353146	-0.783253
H	1.879943	0.828765	-1.700931
H	2.839273	1.313012	1.146878
O	2.342281	-0.630730	0.537140
O	-0.303564	-0.940016	1.476233
O	0.256208	-1.550202	-1.085608
S	-2.231290	-0.040642	-0.610246
C	-2.656313	1.119419	0.737537
H	-2.063622	2.024594	0.659448
H	-2.441717	0.651878	1.690483
H	3.782980	0.706708	-0.221127
H	-3.712142	1.380882	0.690577

S5′ Dianionic Reactant Structure at the Gas-B3LYP/6-31+G(d) level:

C	-1.800268	2.034857	0.573628
S	-1.704121	0.914147	-0.880258
P	-0.841622	-0.879843	0.116269
O	-0.750647	-1.892896	-1.001325
O	0.623780	-0.331065	0.595126
C	1.750835	-0.136759	-0.312369
C	3.003094	0.361326	0.462042
O	4.078763	0.547256	-0.341162
O	-1.655871	-1.096185	1.372844
H	1.974130	-1.086635	-0.812329
H	1.471828	0.603911	-1.074121
H	2.660765	1.292426	1.009807
H	3.160140	-0.395758	1.288545
H	-2.328548	2.949696	0.274606
H	-2.341891	1.539790	1.385392
H	-0.796328	2.294443	0.924532

S5′ Early Transition State (ETS) Structure at the Gas-B3LYP/6-31+G(d) level:

P	0.075683	-0.598737	0.023487
O	0.496474	1.006927	-0.166679
C	1.811121	1.270592	-0.650979
C	2.824204	0.609419	0.303495
H	1.909873	2.369329	-0.697509
H	1.918548	0.849835	-1.663819
H	2.895727	1.273946	1.220490
O	2.423647	-0.649704	0.560210
O	-0.304435	-0.973914	1.430587
O	0.319997	-1.467939	-1.180951
S	-2.307382	0.047165	-0.678600
C	-2.860538	0.880375	0.866517
H	-2.478763	1.909872	0.934576
H	-2.476903	0.318428	1.726353
H	3.840777	0.701715	-0.193778
H	-3.960584	0.918019	0.919452

S5′ Dianionic Reactant Structure at the Gas-M062X/6-31+G(d) level:

C	-1.343118	2.106472	0.559313
S	-1.546817	1.012160	-0.885912
P	-0.937450	-0.839798	0.117437
O	-0.910074	-1.866259	-0.976311
O	0.549196	-0.426402	0.623148
C	1.669044	-0.326905	-0.281903
C	2.886315	0.297158	0.437329
O	3.981212	0.376005	-0.344847
O	-1.795425	-0.954418	1.345087
H	1.924697	-1.329010	-0.648296
H	1.390994	0.297313	-1.142633
H	2.509152	1.291145	0.824849
H	3.018019	-0.320753	1.373083
H	-1.673857	3.115617	0.289798
H	-1.939560	1.724909	1.392733
H	-0.291356	2.131434	0.858444

S5′ Early Transition State (ETS) Structure at the Gas-M062X/6-31+G(d) level:

P	0.008765	-0.596659	0.037596
O	0.451198	0.986904	-0.174879
C	1.740983	1.210196	-0.711951
C	2.765025	0.611013	0.263687
H	1.845446	2.300028	-0.846205
H	1.819364	0.707168	-1.688455
H	2.847792	1.335578	1.129544
O	2.359134	-0.618921	0.603580
O	-0.338120	-0.943571	1.451031
O	0.308740	-1.483157	-1.130744
S	-2.222031	-0.006563	-0.650789
C	-2.655522	0.996934	0.809434
H	-2.101726	1.944103	0.811291
H	-2.380000	0.440882	1.711646
H	3.771752	0.670118	-0.252539
H	-3.732152	1.218131	0.824482

S5′ Dianionic Reactant Structure at the Gas-B3LYP/6-311+G(d,p) level:

C	-1.792478	2.031161	0.581944
S	-1.714114	0.921055	-0.879792
P	-0.840582	-0.883587	0.116141
O	-0.748661	-1.896377	-0.993266
O	0.620824	-0.328676	0.583755
C	1.754024	-0.136999	-0.317038
C	3.000734	0.366866	0.458954
O	4.078729	0.545425	-0.336877
O	-1.647303	-1.099297	1.370061
H	1.983520	-1.086556	-0.809736
H	1.480585	0.597342	-1.083632
H	2.653102	1.298164	0.998093
H	3.147569	-0.381271	1.292264
H	-2.338381	2.936746	0.299522
H	-2.308294	1.520026	1.396441
H	-0.785933	2.297711	0.909073

S5′ Early Transition State (ETS) Structure at the Gas-B3LYP/6-311+G(d,p) level:

P	0.084317	-0.597906	0.011944
O	0.512301	1.002967	-0.149122
C	1.827144	1.279832	-0.625047
C	2.838602	0.598690	0.316157
H	1.926569	2.376001	-0.647354
H	1.938219	0.879473	-1.643189
H	2.913540	1.247468	1.241221
O	2.434065	-0.660903	0.550446
O	-0.305752	-0.986622	1.404479
O	0.322599	-1.442301	-1.202115
S	-2.327742	0.080302	-0.686554
C	-2.890703	0.829064	0.895832
H	-2.573536	1.875701	0.986066
H	-2.447752	0.264649	1.721106
H	3.851844	0.697072	-0.179642
H	-3.985716	0.792761	0.976328

S5′ Dianionic Reactant Structure at the Gas-M062X/6-311+G(d,p) level:

C	-1.323167	2.103621	0.568443
S	-1.541998	1.025157	-0.886506
P	-0.942581	-0.839705	0.116651
O	-0.919488	-1.866481	-0.969392
O	0.543799	-0.432765	0.614253
C	1.670051	-0.335928	-0.285391
C	2.879346	0.300007	0.434537
O	3.980472	0.365321	-0.338192
O	-1.796614	-0.951882	1.340409
H	1.933638	-1.337736	-0.638740
H	1.393953	0.276869	-1.151632
H	2.498410	1.296010	0.801660
H	2.998245	-0.301951	1.377977
H	-1.635092	3.116739	0.305170
H	-1.927653	1.721331	1.392029
H	-0.273529	2.102043	0.865717

S5′ Early Transition State (ETS) Structure at the Gas-M062X/6-311+G(d,p) level:

P	0.010398	-0.609990	0.046178
O	0.440341	0.970933	-0.184539
C	1.725069	1.211444	-0.727042
C	2.759223	0.627434	0.247416
H	1.815171	2.298536	-0.864827
H	1.807662	0.703873	-1.698124
H	2.839314	1.355358	1.105325
O	2.361803	-0.602674	0.596100
O	-0.328642	-0.940512	1.458650
O	0.305559	-1.505234	-1.108962
S	-2.237252	-0.020701	-0.638394
C	-2.613092	1.042362	0.794601
H	-2.006203	1.951863	0.761083
H	-2.360446	0.498371	1.707537
H	3.758465	0.687687	-0.273200
H	-3.673597	1.317822	0.804007

S5′ Dianionic Reactant Structure at the Gas-MP2/6-311+G(d,p) level:

C	-1.258892	2.133437	0.555286
S	-1.534868	1.043042	-0.871514
P	-0.959071	-0.837489	0.112292
O	-0.924426	-1.849134	-0.998579
O	0.533645	-0.440212	0.636423
C	1.663932	-0.367315	-0.269669
C	2.866382	0.300175	0.431593
O	3.978833	0.335382	-0.346274
O	-1.821949	-0.980277	1.336745
H	1.938380	-1.379873	-0.585019
H	1.389502	0.214868	-1.158137
H	2.485024	1.311319	0.753298
H	2.983721	-0.267619	1.396512
H	-1.523398	3.157390	0.269127
H	-1.877468	1.815462	1.398522
H	-0.209169	2.098255	0.855754

S5′ Early Transition State (ETS) Structure at the Gas-MP2/6-311+G(d,p) level:

P	0.049929	-0.636174	0.060966
O	0.410701	0.970344	-0.217149
C	1.700844	1.237081	-0.738278
C	2.728509	0.666681	0.245590
H	1.773769	2.329249	-0.863262
H	1.816642	0.738345	-1.712536
H	2.766839	1.378157	1.120776
O	2.345723	-0.588379	0.559879
O	-0.290356	-0.943539	1.485794
O	0.315799	-1.548316	-1.097323
S	-2.267968	-0.045602	-0.617358
C	-2.579602	1.090125	0.765403
H	-1.916867	1.961249	0.703691
H	-2.372376	0.584999	1.714497
H	3.737948	0.753034	-0.249781
H	-3.620840	1.442997	0.763942

S5′ Dianionic Reactant Structure at the PCM-HF/3-21+G* level:

C	-1.662213	2.105277	0.542333
S	-1.699414	0.878095	-0.810358
P	-0.878652	-0.810953	0.106070
O	-0.862457	-1.859175	-0.976424
O	0.606753	-0.386273	0.506752
C	1.758235	-0.116463	-0.391527
C	2.946254	0.236084	0.499208
O	4.090180	0.542999	-0.320513
O	-1.602703	-1.108900	1.391964
H	1.947813	-1.014115	-0.980691
H	1.492732	0.715406	-1.045603
H	2.663551	1.088609	1.128981
H	3.144418	-0.612523	1.165446
H	-2.085151	3.022599	0.151261
H	-2.255815	1.766892	1.380357
H	-0.644987	2.289320	0.860617

S5′ Early Transition State (ETS) Structure at the PCM-HF/3-21+G* level:

P	-0.026469	-0.576568	0.057378
O	0.439914	0.861549	-0.507717
C	1.815460	1.368801	-0.679835
C	2.675197	0.625138	0.333548
H	1.760935	2.445579	-0.527347
H	2.115339	1.138572	-1.702700
H	2.540534	1.062402	1.330307
O	2.201501	-0.728049	0.285726
O	-0.125906	-0.676475	1.569519
O	0.082622	-1.792423	-0.846517
S	-2.133275	-0.168233	-0.451896
C	-2.561626	1.312366	0.522156
H	-1.977066	2.164305	0.200473
H	-2.388042	1.137516	1.576230
H	3.731571	0.709873	0.058953
H	-3.613061	1.527358	0.370448

S5′ Dianionic Reactant Structure at the PCM-B3LYP/6-31+G(d) level:

C	-1.759179	2.104547	0.559590
S	-1.633321	0.925196	-0.847731
P	-0.861158	-0.847639	0.096010
O	-0.773657	-1.856819	-1.036941
O	0.630085	-0.427526	0.632235
C	1.737219	-0.206652	-0.293348
C	2.935875	0.360884	0.482734
O	4.028019	0.572115	-0.355061
O	-1.661907	-1.159180	1.348045
H	2.003255	-1.172555	-0.766209
H	1.415151	0.506882	-1.079322
H	2.584462	1.301636	0.984948
H	3.158508	-0.360416	1.314043
H	-2.171849	3.033794	0.152099
H	-2.430956	1.715924	1.330762
H	-0.771860	2.304796	0.987156

S5′ Early Transition State (ETS) Structure at the PCM-B3LYP/6-31+G(d) level:

P	0.010988	-0.574352	0.062805
O	0.436180	0.946151	-0.464922
C	1.813207	1.336495	-0.699208
C	2.689053	0.637503	0.330785
H	1.833151	2.442277	-0.629842
H	2.090000	1.023209	-1.727717
H	2.550110	1.142162	1.324019
O	2.295060	-0.697325	0.353347
O	-0.140897	-0.720602	1.578942
O	0.159486	-1.746297	-0.911022
S	-2.168007	-0.163193	-0.508559
C	-2.706183	1.211844	0.587411
H	-2.150595	2.130510	0.369063
H	-2.562402	0.945551	1.640240
H	3.760601	0.779730	0.044250
H	-3.772665	1.392462	0.410158

S5′ Dianionic Reactant Structure at the PCM-M062X/6-31+G(d) level:

C	-1.074282	2.233871	0.565791
S	-1.107679	1.139929	-0.894705
P	-1.019029	-0.756617	0.065890
O	-1.088837	-1.762384	-1.057150
O	0.450519	-0.766657	0.760934
C	1.640633	-0.778409	-0.060210
C	2.601316	0.313030	0.412599
O	3.756569	0.333284	-0.346188
O	-2.005575	-0.793059	1.205160
H	2.103826	-1.780593	0.032790
H	1.372475	-0.607214	-1.122835
H	2.025687	1.277706	0.367401
H	2.792457	0.129939	1.502548
H	-1.019833	3.262517	0.197651
H	-1.981814	2.105067	1.161151
H	-0.191902	2.022528	1.177099

S5′ Early Transition State (ETS) Structure at the PCM-M062X/6-31+G(d) level:

P	0.065901	-0.329257	0.044208
O	-0.768897	1.038794	-0.324660
C	-2.095517	1.219735	0.196276
C	-2.910598	0.010077	-0.237122
H	-2.461394	2.180265	-0.212366
H	-2.036499	1.281349	1.303047
H	-3.147048	0.121180	-1.326559
O	-2.142366	-1.109549	0.028590
O	0.331658	-1.310804	-1.081057
O	0.104546	-0.716555	1.510400
S	1.927332	0.928411	-0.125037
C	3.193737	-0.371452	0.038893
H	3.076644	-1.119217	-0.750818
H	3.122408	-0.863841	1.014199
H	-3.886313	0.027852	0.307064
H	4.181121	0.091442	-0.051555

S5′ Dianionic Reactant Structure at the PCM-B3LYP/6-311+G(d,p) level:

C	-1.729043	2.111529	0.564847
S	-1.641084	0.932114	-0.844275
P	-0.865029	-0.849117	0.096667
O	-0.783187	-1.856816	-1.030452
O	0.625587	-0.428686	0.620416
C	1.737320	-0.209358	-0.300705
C	2.931944	0.354857	0.479500
O	4.026447	0.565613	-0.352331
O	-1.655896	-1.160468	1.348032
H	2.004557	-1.174234	-0.772893
H	1.420855	0.504768	-1.087276
H	2.577503	1.292778	0.982490
H	3.146766	-0.367042	1.310921
H	-2.142883	3.039842	0.164586
H	-2.386011	1.725685	1.345746
H	-0.732932	2.301819	0.967636

S5′ Early Transition State (ETS) Structure at the PCM-B3LYP/6-311+G(d,p) level:

P	0.018319	-0.579861	0.063711
O	0.436621	0.940141	-0.460443
C	1.810780	1.341257	-0.696444
C	2.689261	0.639892	0.327685
H	1.827191	2.445306	-0.619524
H	2.088367	1.035430	-1.725849
H	2.557796	1.144887	1.320359
O	2.289290	-0.692341	0.350399
O	-0.139288	-0.727712	1.572787
O	0.162604	-1.744633	-0.909540
S	-2.176760	-0.159912	-0.509385
C	-2.701970	1.215199	0.590628
H	-2.149553	2.129641	0.362593
H	-2.543193	0.947997	1.637834
H	3.758344	0.778543	0.035622
H	-3.767824	1.392981	0.426636

S5′ Dianionic Reactant Structure at the PCM-M062X/6-311+G(d,p) level:

C	-1.033815	2.233082	0.574404
S	-1.096249	1.152061	-0.894986
P	-1.027642	-0.750529	0.065214
O	-1.108265	-1.755598	-1.051037
O	0.440218	-0.774148	0.753391
C	1.634944	-0.792411	-0.062671
C	2.593030	0.299523	0.410361
O	3.751099	0.316624	-0.343920
O	-2.009933	-0.780293	1.201722
H	2.096590	-1.793442	0.036935
H	1.371255	-0.624222	-1.126254
H	2.016377	1.261557	0.360404
H	2.776097	0.118733	1.500503
H	-0.966401	3.260597	0.213034
H	-1.937881	2.109648	1.171294
H	-0.151323	1.998243	1.171827

S5′ Early Transition State (ETS) Structure at the PCM-M062X/6-311+G(d,p) level:

P	0.064719	-0.329861	0.048230
O	-0.769507	1.037371	-0.312545
C	-2.103683	1.219642	0.190004
C	-2.909262	0.006218	-0.247793
H	-2.467570	2.176003	-0.227384
H	-2.059608	1.283888	1.296448
H	-3.134144	0.111315	-1.338640
O	-2.136768	-1.107290	0.032462
O	0.330648	-1.300771	-1.078822
O	0.106904	-0.722407	1.507681
S	1.932357	0.932911	-0.116352
C	3.189734	-0.378461	0.022096
H	3.050930	-1.115310	-0.770537
H	3.122849	-0.873833	0.993277
H	-3.888608	0.022639	0.286975
H	4.176686	0.077012	-0.078009

S5′ Dianionic Reactant Structure at the PCM-MP2/6-311+G(d,p) level:

C	-1.220981	2.191667	0.546508
S	-1.403572	1.061809	-0.865377
P	-0.973276	-0.793996	0.089801
O	-0.954454	-1.812136	-1.025678
O	0.523693	-0.567232	0.696333
C	1.658300	-0.511202	-0.206137
C	2.759171	0.325297	0.441842
O	3.900727	0.354598	-0.357520
O	-1.868855	-0.980455	1.291231
H	2.013491	-1.543986	-0.391603
H	1.353769	-0.051755	-1.168860
H	2.322997	1.340893	0.623653
H	2.943178	-0.116157	1.454440
H	-1.433194	3.199782	0.178813
H	-1.930926	1.941436	1.338502
H	-0.200871	2.158009	0.935863

S5′ Early Transition State (ETS) Structure at the PCM-MP2/6-311+G(d,p) level:

P	-0.014483	-0.598851	0.063818
O	0.388832	0.892057	-0.534663
C	1.748726	1.333381	-0.715829
C	2.603228	0.660114	0.339007
H	1.730129	2.438691	-0.641580
H	2.081277	1.024558	-1.727962
H	2.369388	1.125877	1.330279
O	2.269600	-0.689942	0.295513
O	-0.103150	-0.677305	1.580652
O	0.129396	-1.807118	-0.849564
S	-2.158370	-0.175632	-0.451085
C	-2.495417	1.302290	0.543824
H	-1.907327	2.151992	0.187582
H	-2.257384	1.120219	1.595431
H	3.677110	0.867298	0.117356
H	-3.558664	1.547993	0.461474

Native Anionic Reactant Structure at the Gas-HF/3-21+G* level:

P	-0.581700	-0.411788	0.226201
O	0.162973	0.886145	-0.422659
C	1.448739	1.420085	-0.027213
C	2.468358	0.343330	0.351359
H	1.303770	2.088314	0.815384
H	1.799332	1.976981	-0.883504
H	2.153718	-0.171268	1.250617
O	2.681827	-0.603837	-0.714646
O	-0.884575	-0.113680	1.658934
O	-1.938378	-0.368975	-0.639066
O	0.209228	-1.622806	-0.159915
C	-2.940755	0.659883	-0.464188
H	-2.542923	1.615189	-0.781940
H	-3.238887	0.713619	0.574037
H	1.898324	-1.198518	-0.759984
H	3.421781	0.822151	0.537949
H	-3.776266	0.375790	-1.086498

Native Anionic Reactant Structure at the Gas-B3LYP/6-31+G(d) level:

P	-0.569740	-0.401447	0.241981
O	0.181838	0.871082	-0.551388
C	1.406735	1.400419	-0.056590
C	2.449943	0.345169	0.337835
H	1.215330	2.046190	0.817339
H	1.801831	2.019839	-0.872520
H	2.137695	-0.144481	1.271905
O	2.689265	-0.619530	-0.670432
O	-0.862216	0.002853	1.664704
O	-1.958363	-0.406293	-0.656979
O	0.182038	-1.667599	-0.108850
C	-2.901933	0.633246	-0.437502
H	-2.516083	1.596810	-0.799703
H	-3.148032	0.725423	0.627381
H	1.869694	-1.176498	-0.678967
H	3.399876	0.865575	0.531097
H	-3.803182	0.371734	-1.005145

Native Anionic Reactant Structure at the Gas-M062X/6-31+G(d) level:

P	-0.555851	-0.413052	0.233986
O	0.170566	0.820262	-0.609996
C	1.342573	1.392086	-0.061731
C	2.384066	0.352366	0.354594
H	1.087933	2.012865	0.811298
H	1.756492	2.030838	-0.851225
H	2.036615	-0.165022	1.260281
O	2.665831	-0.572703	-0.667632
O	-0.802924	0.054105	1.636502
O	-1.957371	-0.441747	-0.614492
O	0.186772	-1.681126	-0.081309
C	-2.832385	0.650675	-0.422950
H	-2.382704	1.578222	-0.800468
H	-3.071572	0.777361	0.638848
H	1.870168	-1.152849	-0.704359
H	3.317472	0.877571	0.599497
H	-3.745164	0.435702	-0.987735

Native Anionic Reactant Structure at the Gas-B3LYP/6-311+G(d,p) level:

P	-0.570806	-0.405651	0.243576
O	0.175790	0.885856	-0.518344
C	1.411257	1.402130	-0.039029
C	2.450836	0.338122	0.333382
H	1.239879	2.040344	0.841776
H	1.800104	2.024738	-0.852098
H	2.140031	-0.159897	1.260821
O	2.682895	-0.613335	-0.686489
O	-0.874395	-0.031510	1.666505
O	-1.952043	-0.399376	-0.659515
O	0.188251	-1.654737	-0.125527
C	-2.896384	0.640546	-0.450269
H	-2.511935	1.598092	-0.822228
H	-3.138514	0.744154	0.612297
H	1.872346	-1.171474	-0.693960
H	3.399554	0.853725	0.532473
H	-3.797621	0.375103	-1.010270

Native Anionic Reactant Structure at the Gas-M062X/6-311+G(d,p) level:

P	-0.556847	-0.418671	0.233213
O	0.164254	0.828928	-0.589751
C	1.342426	1.393828	-0.048099
C	2.383939	0.349325	0.352569
H	1.097204	2.002766	0.832833
H	1.751442	2.037973	-0.831805
H	2.036256	-0.176153	1.250655
O	2.665723	-0.564294	-0.678951
O	-0.802524	0.027039	1.638063
O	-1.957797	-0.437481	-0.609356
O	0.187987	-1.674257	-0.098405
C	-2.828052	0.660791	-0.430067
H	-2.375000	1.577879	-0.822007
H	-3.058829	0.803852	0.629511
H	1.880769	-1.146451	-0.716670
H	3.313180	0.873107	0.604417
H	-3.743355	0.443960	-0.984341

Native Anionic Reactant Structure at the Gas-MP2/6-311+G(d,p) level:

P	-0.558174	-0.404597	0.242948
O	0.165669	0.849993	-0.590578
C	1.362537	1.394345	-0.056397
C	2.398130	0.342609	0.345919
H	1.141974	2.017354	0.824081
H	1.777334	2.023454	-0.851440
H	2.058517	-0.168607	1.255167
O	2.668500	-0.592696	-0.677855
O	-0.839847	0.048013	1.646445
O	-1.947558	-0.446537	-0.635986
O	0.206537	-1.661715	-0.073905
C	-2.852046	0.629005	-0.440583
H	-2.390702	1.583659	-0.719551
H	-3.178215	0.685386	0.603106
H	1.864633	-1.154182	-0.685044
H	3.334337	0.867155	0.578767
H	-3.713399	0.442522	-1.087903

S3′ Anionic Reactant Structure at the Gas-HF/3-21+G* level:

P	-0.681234	-0.494240	0.117185
S	0.275307	1.282405	-0.533976
C	1.840058	1.225701	0.419479
C	2.503198	-0.156386	0.568957
H	1.663136	1.626577	1.409821
H	2.514804	1.887266	-0.108830
H	1.924056	-0.773956	1.241026
O	2.696321	-0.835837	-0.688355
O	-0.876430	-0.443444	1.597302
O	-2.102965	-0.271810	-0.618006
O	0.041089	-1.636411	-0.522996
C	-3.216900	0.447648	-0.030310
H	-3.016950	1.511636	-0.047196
H	-3.370686	0.123537	0.988143
H	1.862130	-1.286928	-0.937436
H	3.490087	-0.014477	0.991860
H	-4.075215	0.219708	-0.643859

S3′ Anionic Reactant Structure at the Gas-B3LYP/6-31+G(d) level:

P	-0.703508	-0.519049	0.128875
S	0.290731	1.326809	-0.510027
C	1.893130	1.223378	0.408578
C	2.525007	-0.173798	0.542077
H	1.761457	1.639592	1.415690
H	2.567794	1.881204	-0.152372
H	1.939353	-0.765411	1.258709
O	2.678555	-0.876019	-0.674897
O	-0.924275	-0.493606	1.619690
O	-2.140881	-0.270101	-0.664986
O	0.001141	-1.658305	-0.574987
C	-3.145380	0.508984	-0.021066
H	-3.389603	0.100244	0.965688
H	-4.028608	0.477956	-0.669429
H	1.787880	-1.257646	-0.872042
H	3.532122	-0.038359	0.965230
H	-2.822340	1.552081	0.099745

S3′ Anionic Reactant Structure at the Gas-M062X/6-31+G(d) level:

P	-0.678665	-0.527971	0.107894
S	0.277996	1.280051	-0.598866
C	1.774812	1.220905	0.454682
C	2.435313	-0.158170	0.583596
H	1.524972	1.584938	1.457568
H	2.475180	1.922680	-0.011202
H	1.819149	-0.789747	1.236346
O	2.677561	-0.796761	-0.644939
O	-0.834908	-0.434043	1.594660
O	-2.135606	-0.317204	-0.622424
O	0.011770	-1.676235	-0.570176
C	-3.065407	0.522907	0.037875
H	-2.667939	1.540584	0.143860
H	-3.301790	0.134484	1.033408
H	1.821401	-1.205556	-0.902083
H	3.408509	-0.015712	1.073929
H	-3.966291	0.547170	-0.582278

S3′ Anionic Reactant Structure at the Gas-B3LYP/6-311+G(d,p) level:

P	-0.705194	-0.516214	0.135058
S	0.298983	1.337855	-0.493838
C	1.902481	1.212277	0.417170
C	2.525531	-0.188090	0.530648
H	1.773212	1.614599	1.426783
H	2.574567	1.872917	-0.137502
H	1.936554	-0.782486	1.238413
O	2.674873	-0.875864	-0.693147
O	-0.944582	-0.493779	1.617208
O	-2.132403	-0.269417	-0.669788
O	0.006545	-1.647222	-0.560687
C	-3.155314	0.500293	-0.045266
H	-3.374854	0.123111	0.957106
H	-4.042519	0.419490	-0.678691
H	1.791513	-1.257913	-0.886669
H	3.529521	-0.063666	0.958757
H	-2.865476	1.554840	0.033338

S3′ Anionic Reactant Structure at the Gas-M062X/6-311+G(d,p) level:

P	-0.678208	-0.530806	0.107392
S	0.280345	1.284419	-0.597300
C	1.767410	1.214984	0.468048
C	2.431560	-0.162699	0.580892
H	1.500792	1.556758	1.470979
H	2.464453	1.927032	0.020254
H	1.813799	-0.801051	1.221148
O	2.682510	-0.786131	-0.652930
O	-0.832997	-0.437648	1.589436
O	-2.134957	-0.323138	-0.615732
O	0.012501	-1.672199	-0.568369
C	-3.066692	0.525180	0.031332
H	-2.671621	1.543253	0.118212
H	-3.296754	0.155173	1.033109
H	1.837038	-1.195851	-0.914825
H	3.397964	-0.022672	1.079657
H	-3.968191	0.536875	-0.583493

S3′ Anionic Reactant Structure at the Gas-MP2/6-311+G(d,p) level:

P	-0.680361	-0.522193	0.125523
S	0.284022	1.296188	-0.563679
C	1.791760	1.212739	0.456444
C	2.454156	-0.168628	0.559336
H	1.573152	1.560985	1.472311
H	2.490526	1.912036	-0.015112
H	1.851967	-0.802215	1.220185
O	2.672289	-0.809683	-0.678733
O	-0.896797	-0.431553	1.607204
O	-2.117818	-0.316708	-0.658386
O	0.033259	-1.668456	-0.536471
C	-3.081066	0.506685	-0.012080
H	-2.690436	1.517504	0.154251
H	-3.374300	0.085941	0.953712
H	1.804344	-1.206162	-0.893555
H	3.436246	-0.026804	1.030147
H	-3.947005	0.559028	-0.677010

S5′ Anionic Reactant Structure at the Gas-HF/3-21+G* level:

P	-0.290349	-0.340758	0.376114
O	0.402973	0.769739	-0.593649
C	1.692536	1.397406	-0.362261
C	2.737067	0.441194	0.217359
H	1.553787	2.233060	0.314542
H	2.007122	1.751402	-1.331974
H	2.453581	0.138175	1.217274
O	2.939756	-0.717817	-0.616815
O	-0.477653	0.270588	1.725877
O	0.466600	-1.624984	0.200748
S	-2.130313	-0.580534	-0.582741
C	-2.908792	1.010750	-0.152018
H	-2.381253	1.827406	-0.624675
H	-2.897637	1.149438	0.918671
H	2.169173	-1.319466	-0.514120
H	3.687803	0.957166	0.265222
H	-3.930596	0.986427	-0.510556

S5′ Anionic Reactant Structure at the Gas-B3LYP/6-31+G(d) level:

P	-0.261929	-0.322682	0.407737
O	0.433399	0.742864	-0.685448
C	1.673163	1.374767	-0.365033
C	2.753189	0.428373	0.178104
H	1.508618	2.179725	0.370115
H	2.013467	1.820111	-1.308382
H	2.502743	0.139937	1.209490
O	2.955050	-0.722062	-0.622415
O	-0.468254	0.386350	1.722745
O	0.476216	-1.643294	0.286485
S	-2.152802	-0.607909	-0.583638
C	-2.968703	0.984273	-0.167350
H	-2.511379	1.811930	-0.718194
H	-2.884575	1.172741	0.905726
H	2.147729	-1.274234	-0.476169
H	3.703497	0.981639	0.205136
H	-4.023517	0.899575	-0.450816

S5′ Anionic Reactant Structure at the Gas-M062X/6-31+G(d) level:

P	-0.254712	-0.343079	0.382489
O	0.416897	0.690661	-0.731041
C	1.606979	1.365567	-0.353377
C	2.676794	0.431752	0.213512
H	1.379435	2.145289	0.389088
H	1.977422	1.834592	-1.272173
H	2.373741	0.098591	1.216336
O	2.931941	-0.672581	-0.620986
O	-0.416840	0.400900	1.673264
O	0.467363	-1.660417	0.273072
S	-2.156079	-0.610816	-0.538418
C	-2.848912	1.030577	-0.154141
H	-2.308739	1.808502	-0.699894
H	-2.768256	1.220183	0.918015
H	2.146848	-1.255770	-0.516719
H	3.612352	0.998607	0.312012
H	-3.898907	1.033378	-0.459752

S5′ Anionic Reactant Structure at the Gas-B3LYP/6-311+G(d,p) level:

P	-0.261935	-0.329050	0.409123
O	0.426270	0.758295	-0.661033
C	1.675673	1.378847	-0.361309
C	2.751402	0.427732	0.175843
H	1.530482	2.187382	0.370811
H	2.010193	1.816064	-1.307526
H	2.497672	0.138876	1.203892
O	2.952771	-0.719183	-0.626647
O	-0.474892	0.352685	1.730890
O	0.483114	-1.636702	0.267257
S	-2.154965	-0.601286	-0.594981
C	-2.960654	0.989797	-0.159511
H	-2.512361	1.812747	-0.718212
H	-2.851191	1.170844	0.909448
H	2.155855	-1.273825	-0.478188
H	3.698886	0.980980	0.209122
H	-4.017692	0.904249	-0.420368

S5′ Anionic Reactant Structure at the Gas-M062X/6-311+G(d,p) level:

P	-0.256662	-0.362037	0.382056
O	0.402257	0.706484	-0.701344
C	1.596407	1.374789	-0.327188
C	2.670659	0.432283	0.213455
H	1.378859	2.136013	0.433781
H	1.957325	1.861126	-1.237443
H	2.367902	0.076814	1.206067
O	2.930997	-0.651466	-0.645056
O	-0.410694	0.340912	1.691112
O	0.469787	-1.666148	0.231998
S	-2.164913	-0.599139	-0.541886
C	-2.813731	1.059484	-0.154520
H	-2.250401	1.815158	-0.702300
H	-2.722471	1.241577	0.915443
H	2.159786	-1.241961	-0.549483
H	3.599758	1.002160	0.326170
H	-3.861001	1.088293	-0.457057

S5′ Anionic Reactant Structure at the Gas-MP2/6-311+G(d,p) level:

P	-0.260058	-0.378126	0.403506
O	0.373371	0.759452	-0.640388
C	1.590222	1.394796	-0.268676
C	2.676193	0.422913	0.193870
H	1.411880	2.125019	0.535151
H	1.929502	1.917959	-1.168742
H	2.409044	0.030253	1.182552
O	2.905053	-0.633905	-0.715835
O	-0.423194	0.252795	1.755732
O	0.491803	-1.666937	0.178556
S	-2.151207	-0.587928	-0.557611
C	-2.791949	1.070789	-0.194757
H	-2.210481	1.827421	-0.725672
H	-2.744801	1.266288	0.877922
H	2.121392	-1.209062	-0.600577
H	3.612336	0.987783	0.292358
H	-3.831748	1.110851	-0.530960

Native Anionic Reactant Structure at the PCM-HF/3-21+G* level:

P	-0.808585	-0.546789	-0.082008
O	0.371934	0.508046	0.182421
C	1.546911	0.345494	1.056739
C	2.716372	-0.179717	0.249298
H	1.302858	-0.339489	1.869302
H	1.752238	1.337790	1.448945
H	2.482172	-1.145316	-0.197384
O	3.106080	0.763261	-0.797460
O	-1.273001	-1.112195	1.234305
O	-1.921954	0.422817	-0.699017
O	-0.416717	-1.518192	-1.160831
C	-2.599874	1.501431	0.034963
H	-1.865855	2.216060	0.383984
H	-3.147758	1.080997	0.868152
H	2.383571	0.860132	-1.490685
H	3.584176	-0.281305	0.898859
H	-3.273816	1.959821	-0.672389

Native Anionic Reactant Structure at the PCM-B3LYP/6-31+G(d) level:

P	0.954432	-0.516506	0.131011
O	-0.673648	-0.526594	0.302138
C	-1.540302	-0.189521	-0.810811
C	-2.966406	-0.123081	-0.300596
H	-1.459413	-0.972386	-1.588963
H	-1.234415	0.785023	-1.236005
H	-3.238029	-1.081761	0.185972
O	-3.195740	0.972791	0.596528
O	1.376994	-1.130612	-1.191282
O	1.178893	1.121311	0.074740
O	1.518318	-1.071942	1.424880
C	2.481704	1.632204	-0.259288
H	2.780833	1.307961	-1.264596
H	3.231773	1.303353	0.473597
H	-2.653091	0.808230	1.431025
H	-3.637919	0.035658	-1.164047
H	2.405279	2.724259	-0.234015

Native Anionic Reactant Structure at the PCM-M062X/6-31+G(d) level:

P	0.649998	0.484758	0.185028
O	-0.263893	-0.663401	-0.543338
C	-1.353973	-1.272739	0.164571
C	-2.470990	-0.282759	0.433986
H	-0.991322	-1.705158	1.115548
H	-1.712714	-2.082320	-0.493736
H	-2.117133	0.517541	1.115571
O	-2.985788	0.280026	-0.766251
O	0.829282	0.130318	1.639647
O	2.035098	0.255923	-0.641842
O	0.159835	1.855665	-0.201166
C	2.756382	-0.960339	-0.430155
H	2.127115	-1.826751	-0.669588
H	3.098644	-1.028194	0.609042
H	-2.253889	0.832373	-1.184439
H	-3.304647	-0.814050	0.926964
H	3.619184	-0.938024	-1.101583

Native Anionic Reactant Structure at the PCM-B3LYP/6-311+G(d,p) level:

P	0.954022	-0.520411	0.131181
O	-0.671367	-0.539943	0.289414
C	-1.542660	-0.194145	-0.817404
C	-2.961573	-0.117160	-0.297560
H	-1.474614	-0.975348	-1.597035
H	-1.231757	0.777552	-1.243018
H	-3.235975	-1.075106	0.185914
O	-3.174530	0.976400	0.604219
O	1.386412	-1.120635	-1.188637
O	1.172544	1.115173	0.086394
O	1.509915	-1.080468	1.419761
C	2.463388	1.648080	-0.258418
H	2.751579	1.345314	-1.271289
H	3.228026	1.317655	0.455302
H	-2.626312	0.809079	1.423964
H	-3.636627	0.045885	-1.156156
H	2.376623	2.736273	-0.214306

Native Anionic Reactant Structure at the PCM-M062X/6-311+G(d,p) level:

P	0.647277	0.484383	0.184376
O	-0.258830	-0.669952	-0.536878
C	-1.357257	-1.277789	0.160632
C	-2.469208	-0.284530	0.431778
H	-1.003258	-1.714261	1.111983
H	-1.717003	-2.081196	-0.502619
H	-2.112143	0.508315	1.118629
O	-2.978542	0.288155	-0.765272
O	0.825456	0.138028	1.636549
O	2.033468	0.258429	-0.634197
O	0.151454	1.846178	-0.206063
C	2.763011	-0.954580	-0.429807
H	2.140574	-1.821317	-0.677658
H	3.100227	-1.028335	0.608917
H	-2.245223	0.825334	-1.179922
H	-3.303005	-0.816398	0.921767
H	3.627356	-0.923201	-1.095458

Native Anionic Reactant Structure at the PCM-MP2/6-311+G(d,p) level:

P	0.683427	0.506476	0.171703
O	-0.291081	-0.633990	-0.505447
C	-1.369063	-1.214237	0.253238
C	-2.512220	-0.238954	0.448634
H	-1.002282	-1.562337	1.236635
H	-1.710482	-2.076761	-0.343871
H	-2.173780	0.631558	1.044058
O	-3.068611	0.192774	-0.795770
O	0.871797	0.198624	1.637551
O	2.048983	0.187841	-0.670807
O	0.250407	1.883324	-0.263562
C	2.726988	-1.053443	-0.422978
H	2.049254	-1.901696	-0.575065
H	3.125506	-1.078481	0.597149
H	-2.335157	0.663826	-1.284191
H	-3.319784	-0.752444	1.001268
H	3.549132	-1.109591	-1.140617

S3′ Anionic Reactant Structure at the PCM-HF/3-21+G* level:

P	0.891734	0.581646	0.043080
S	-0.383770	-1.009205	-0.454848
C	-1.731720	-0.857656	0.779693
C	-2.714132	0.283151	0.520766
H	-1.294250	-0.745423	1.766429
H	-2.258478	-1.807689	0.745699
H	-2.205691	1.245866	0.493374
O	-3.465006	0.087974	-0.718196
O	1.019068	0.674151	1.539655
O	2.257594	0.045591	-0.605723
O	0.505270	1.824987	-0.710791
C	3.154853	-0.975170	-0.039362
H	2.639340	-1.926001	0.001041
H	3.467690	-0.669618	0.949574
H	-2.911420	0.293814	-1.533033
H	-3.459720	0.293474	1.313800
H	3.997428	-1.025421	-0.711650

S3′ Anionic Reactant Structure at the PCM-B3LYP/6-31+G(d) level:

C	2.009120	2.084369	-0.123170
O	1.611063	1.018670	0.760650
P	1.388997	-0.510879	0.179762
O	1.150110	-1.358606	1.412929
S	-0.397119	-0.386811	-1.003669
C	-1.692855	-0.034764	0.273371
C	-3.058645	0.067006	-0.409108
O	-4.097050	0.297893	0.553506
O	2.477356	-0.859671	-0.818635
H	-1.695486	-0.848005	1.011228
H	-1.447941	0.911701	0.777484
H	-3.052791	0.872406	-1.169679
H	-3.311808	-0.885166	-0.907879
H	2.079388	2.986526	0.493309
H	2.983682	1.867264	-0.577154
H	1.258709	2.235140	-0.910866
H	-3.972354	1.226348	0.931681

S3′ Anionic Reactant Structure at the PCM-M062X/6-31+G(d) level:

P	0.813184	0.576758	0.077707
S	-0.349261	-1.068853	-0.639009
C	-1.699452	-1.078902	0.601485
C	-2.562651	0.176829	0.608739
H	-1.261633	-1.235316	1.596981
H	-2.310284	-1.956515	0.343499
H	-1.957337	1.057638	0.899856
O	-3.225374	0.412404	-0.625318
O	0.874512	0.501097	1.581950
O	2.257250	0.185623	-0.579530
O	0.385614	1.850225	-0.604843
C	3.046855	-0.838450	0.032644
H	2.485033	-1.779888	0.083728
H	3.350707	-0.535477	1.040553
H	-2.535329	0.680171	-1.309704
H	-3.355001	0.039960	1.367080
H	3.929718	-0.971945	-0.598733

S3′ Anionic Reactant Structure at the PCM-B3LYP/6-311+G(d,p) level:

C	2.009891	2.086526	-0.131654
O	1.605818	1.020314	0.748680
P	1.389074	-0.511044	0.183204
O	1.152665	-1.347422	1.417255
S	-0.401658	-0.398386	-1.006982
C	-1.691914	-0.028920	0.270070
C	-3.058963	0.062394	-0.405423
O	-4.091796	0.306746	0.558137
O	2.477789	-0.861161	-0.805520
H	-1.686988	-0.831467	1.015742
H	-1.442073	0.923007	0.755335
H	-3.055064	0.855529	-1.177040
H	-3.311263	-0.895220	-0.891528
H	2.070983	2.989112	0.480799
H	2.987926	1.872862	-0.574605
H	1.269780	2.233977	-0.926751
H	-3.952770	1.224221	0.935320

S3′ Anionic Reactant Structure at the PCM-M062X/6-311+G(d,p) level:

P	0.813252	0.578078	0.071768
S	-0.354446	-1.073436	-0.637936
C	-1.696811	-1.070547	0.610954
C	-2.557469	0.184968	0.609904
H	-1.249529	-1.214454	1.601479
H	-2.306426	-1.949243	0.362875
H	-1.946928	1.065947	0.884275
O	-3.229283	0.405491	-0.621208
O	0.872632	0.510919	1.571587
O	2.256235	0.180429	-0.575189
O	0.390537	1.844655	-0.614482
C	3.049248	-0.839275	0.041231
H	2.479515	-1.771462	0.125394
H	3.377215	-0.518317	1.034036
H	-2.547139	0.647891	-1.310179
H	-3.340606	0.058323	1.378064
H	3.915474	-0.997704	-0.603682

S3′ Anionic Reactant Structure at the PCM-MP2/6-311+G(d,p) level:

P	0.826287	0.577571	0.073448
S	-0.367059	-1.059388	-0.630483
C	-1.695524	-1.048637	0.618134
C	-2.578098	0.193118	0.607852
H	-1.253116	-1.172354	1.616044
H	-2.305474	-1.934445	0.386494
H	-1.979701	1.090285	0.854769
O	-3.278488	0.382217	-0.622312
O	0.907253	0.500453	1.577736
O	2.261002	0.160352	-0.602787
O	0.415804	1.857816	-0.609397
C	3.058785	-0.850703	0.035479
H	2.483670	-1.775072	0.166056
H	3.415423	-0.500406	1.009129
H	-2.593158	0.583242	-1.321100
H	-3.352487	0.064763	1.385911
H	3.907948	-1.038727	-0.626004

S5′ Anionic Reactant Structure at the PCM-HF/3-21+G* level:

P	-0.735414	-0.845502	0.117580
O	0.814574	-0.461321	-0.028532
C	1.587484	0.554313	0.706801
C	3.047341	0.265993	0.439724
H	1.364154	0.470794	1.769991
H	1.303333	1.536764	0.333463
H	3.296220	-0.751683	0.738242
O	3.381321	0.462457	-0.968669
O	-1.110290	-0.859957	1.574349
O	-0.948762	-2.077806	-0.717567
S	-1.799712	0.660577	-0.870642
C	-1.944674	1.984148	0.381086
H	-0.975226	2.378139	0.649796
H	-2.449635	1.616630	1.262356
H	2.923598	-0.214694	-1.554857
H	3.664210	0.971352	0.994009
H	-2.535702	2.772277	-0.068757

S5′ Anionic Reactant Structure at the PCM-B3LYP/6-31+G(d) level:

C	-1.813326	2.099270	0.558567
S	-1.670502	0.929067	-0.854308
P	-0.916734	-0.843561	0.092627
O	-0.806447	-1.853688	-1.034720
O	0.581557	-0.420278	0.639783
C	1.676479	-0.229902	-0.282187
C	2.847649	0.321066	0.519005
O	3.937357	0.495799	-0.398360
O	-1.710398	-1.149698	1.347617
H	1.943005	-1.196970	-0.746173
H	1.382829	0.484670	-1.074937
H	2.567513	1.288139	0.981323
H	3.123511	-0.390572	1.322238
H	-2.213399	3.033352	0.150439
H	-2.499982	1.709851	1.315456
H	-0.832761	2.291509	1.004200
H	4.726943	0.848681	0.120106

S5′ Anionic Reactant Structure at the PCM-M062X/6-31+G(d) level:

P	-0.801605	-0.872783	0.006896
O	0.832819	-0.833124	-0.021220
C	1.540944	0.026300	0.883515
C	2.964793	0.136539	0.384841
H	1.516328	-0.405468	1.901667
H	1.071403	1.030093	0.898128
H	3.417774	-0.872828	0.325421
O	3.038682	0.791660	-0.876209
O	-1.281723	-0.926500	1.433580
O	-1.181228	-1.923233	-1.003546
S	-1.390028	0.997329	-0.834229
C	-1.764513	1.992364	0.650072
H	-0.861217	2.194110	1.230322
H	-2.497460	1.476028	1.272611
H	2.537950	0.229330	-1.545531
H	3.548491	0.744828	1.097881
H	-2.184488	2.936752	0.292308

S5′ Anionic Reactant Structure at the PCM-B3LYP/6-311+G(d,p) level:

C	-1.783577	2.106967	0.561685
S	-1.678334	0.934669	-0.851747
P	-0.920096	-0.844927	0.094249
O	-0.815968	-1.854534	-1.026476
O	0.577620	-0.420174	0.627876
C	1.677743	-0.237225	-0.289063
C	2.840309	0.322450	0.513454
O	3.938144	0.486365	-0.394329
O	-1.703652	-1.149726	1.348873
H	1.949673	-1.207086	-0.741284
H	1.389370	0.468084	-1.090517
H	2.553915	1.292771	0.961590
H	3.105658	-0.379480	1.326868
H	-2.185992	3.038980	0.159380
H	-2.454800	1.720846	1.329535
H	-0.793753	2.290829	0.981677
H	4.714704	0.845643	0.122949

S5′ Anionic Reactant Structure at the PCM-M062X/6-311+G(d,p) level:

P	-0.800908	-0.873161	-0.001893
O	0.829865	-0.835271	-0.019054
C	1.546193	0.014259	0.889959
C	2.963732	0.130129	0.381319
H	1.531641	-0.429964	1.901954
H	1.075945	1.016665	0.920736
H	3.411300	-0.878908	0.301740
O	3.029240	0.806292	-0.868376
O	-1.286390	-0.936650	1.417433
O	-1.178996	-1.915590	-1.012913
S	-1.374995	1.013034	-0.830525
C	-1.779564	1.974019	0.668221
H	-0.897246	2.109858	1.293020
H	-2.563552	1.471465	1.232419
H	2.506180	0.271956	-1.530414
H	3.553465	0.721765	1.102085
H	-2.136108	2.945350	0.321544

S5′ Anionic Reactant Structure at the PCM-MP2/6-311+G(d,p) level:

P	-0.695616	-0.793049	-0.151475
O	0.929956	-0.680484	-0.321427
C	1.731924	-0.310678	0.820707
C	3.104246	0.059037	0.310575
H	1.802539	-1.167810	1.516084
H	1.273987	0.553446	1.339060
H	3.528539	-0.789366	-0.260960
O	3.085510	1.245173	-0.486693
O	-1.057206	-1.299118	1.223707
O	-1.191262	-1.515126	-1.380135
S	-1.190309	1.285510	-0.264876
C	-2.837765	1.211916	0.499050
H	-2.766356	0.877936	1.535554
H	-3.503317	0.548128	-0.058342
H	2.506727	1.046470	-1.276442
H	3.757115	0.268058	1.176722
H	-3.246467	2.225521	0.472848