Effects of Substitution of OH Group by F Atom for Conformational Preferences of Fluorine Substituted Analogues of (R,R)-Tartaric Acid, Its Dimethyl Diester, Diamide and N,N,N',N'-tetramethyl Diamide. Ab Initio Conformational Analysis

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In Tables **S1-S8** are presented the following parameters: MP2 - energy calculated at MP2/6-311++G**//RHF/6-31G* level in kcal/mol, Cor - correlation energy in kcal/mol, 6-311 - energy calculated with 6-311++G** basis set in kcal/mol, 6-31 - energy calculated at RHF/6-31G* level in kcal/mol, μ - dipole momentum in Debyes, CCCC - torsion angle describing conformation of the main carbon chain C_{sp2}–C_{sp3}–C_{sp3}–C_{sp2} in °, FCCO torsion anlges between atoms F–C_{sp3}–C_{sp2}=O in °, HOCC torsion angles H–O–C_{sp2}–C_{sp3} in °, ω - structural degeneracy of the conformer, ZPE - zero point energy calculated with unscaled frequencies in kcal/mol, TCG - thermal correction to Gibss free energy in kcal/mol, % - per cent of the conformer as calculated with unscaled frequencies, ZPE^S zero point energy calculated with scaled frequencies in kcal/mol, TCG^S thermal correction to Gibbs free energy calculated with scaled frequencies in kcal/mol, $\%^S$ - per cent of the conformer as calculated with scaled frequencies. Also Gibbs free energies of solvation and per cents of conformers calculated with AM1-SM5.4 for water (ASM-w and $\%^{Aw}$) and chloroform (AMS-c and $\%^{Ac}$) as well as with PM3-SM5.4 for water (PSM-w and $\%^{Pw}$) and chloroform (PSM-c and $\%^{Pc}$).

Table S1. Selected energetical and geometrical parameters for conformers of (S,S)-2,3-dideoxy-2,3-difluorotartaric acid - FTA.

Conform	MP2	Cor	6-311	6-31	μ	CCCC	FCCO	FCCO	HOCC	HOCC	ω	ZPE	TCG	ZPE^S	TCG^S
Tss	0.00	0.00	0.00	0.00	4.61	169.5	-2.0	-2.0	-179.8	-179.8	1	0.00	0.00	0.00	0.00
Tas	0.07	0.54	-0.48	-0.56	2.83	175.8	178.3	-2.7	-180.0	179.7	2	0.08	-0.05	0.08	-0.06
Taa	0.14	1.09	-0.95	-1.16	0.26	-178.0	174.4	174.4	-179.3	-179.3	1	0.17	-0.09	0.15	-0.11
*Tas**	0.76	-0.33	1.10	1.20	3.72	176.2	-177.8	-2.1	3.0	179.3	2	0.10	0.07	0.09	0.06
*Taa**	0.91	0.23	0.68	0.61	3.03	-178.0	179.0	171.2	3.2	-178.7	2	0.19	0.05	0.17	0.03
G-as	1.60	-0.76	2.36	2.36	3.46	-54.9	-150.5	27.5	179.0	-174.5	2	0.02	-0.38	0.02	-0.39
G-aa	1.73	-0.42	2.16	2.12	1.28	-51.8	-147.0	-147.0	177.8	177.8	1	0.05	-0.56	0.04	-0.57
G-ss	1.81	-0.97	2.78	2.86	3.67	-57.0	26.3	26.3	-177.4	-177.4	1	0.00	-0.15	0.00	-0.16
G-p.+p+	1.88	0.88	0.99	0.89	1.94	-68.5	110.4	110.4	177.8	177.8	1	0.13	-0.45	0.12	-0.47
*Taa***	2.03	-0.63	2.66	2.76	1.83	-178.6	175.5	175.5	3.0	3.0	1	0.20	0.25	0.19	0.24
G-ap-	2.44	0.22	2.22	2.09	2.83	-60.2	148.3	-103.2	-178.7	-178.2	2	0.05	-0.18	0.04	-0.19
G+ss	2.53	-0.73	3.26	2.52	1.08	52.4	22.7	22.7	-175.8	-175.8	1	0.06	-0.17	0.05	-0.18
G+aa	2.78	0.34	2.45	1.57	0.07	45.1	152.6	152.6	-178.9	-178.9	1	0.06	-0.02	0.06	-0.02
G+as	3.01	-0.61	3.62	2.80	2.40	58.3	-145.3	20.6	176.6	-177.2	2	0.05	-0.22	0.05	-0.23
G+p+s	3.02	-0.11	3.13	2.49	2.62	42.2	138.9	-20.1	-178.8	178.6	2	0.02	0.07	0.02	0.07
G+ss	3.03	-0.65	3.67	3.36	0.63	36.9	-19.0	-19.0	177.7	177.7	1	-0.07	-0.08	-0.06	-0.07
*G-ap+**	3.21	-0.75	3.96	3.86	0.99	-69.1	159.8	66.8	5.8	-179.4	2	0.16	0.07	0.15	0.06
*G-ap-**	3.47	-0.82	4.28	4.25	2.10	-60.1	170.7	-113.5	3.3	180.0	2	0.08	0.06	0.07	0.06
G+aa	3.67	-0.47	4.15	3.18	1.20	62.2	-149.3	-149.3	178.6	178.6	1	0.08	-0.18	0.08	-0.19
G-p.-p-	3.76	-0.57	4.33	4.95	2.89	-55.6	-82.3	-82.2	-178.2	-178.2	1	-0.02	-0.83	-0.02	-0.84
*G+aa**	3.87	-0.49	4.35	3.64	3.39	43.5	174.1	147.6	11.2	-179.5	2	0.07	0.08	0.06	0.08
*G+as**	4.40	-1.07	5.47	5.10	4.31	35.0	167.7	-20.3	8.1	179.7	2	0.00	0.12	0.00	0.12
*G+aa***	5.26	-1.31	6.57	6.17	4.13	38.5	169.4	169.4	10.4	10.4	1	0.05	0.07	0.04	0.07

^{S} means calculated with scaled frequencies. Absolute energies (in Hartrees): MP2: -654.0888036479; Cor: -1.743218076; 6-311++G**: -652.345585572; 6-31G*: -652.144610496; ZPE: 0.099097; TCG: 0.063366; ZPE^S: 0.090525; TCG^S 0.054198; and T: 298.15 K; p: 1 atm.

Table S2. Selected energetical and geometrical parameters for conformers of (S,S)-2,3-dideoxy-2,3-difluorotartaric acid diamide FAM

Conform	MP2	Cor	6-311	6-31	μ	CCCC	FCCO	FCCO	ω	ZPE	TCG	ZPE^S	TCG^S
Taa	0.00	0.00	0.00	0.00	3.53	-176.8	175.6	175.6	1	0.00	0.00	0.00	0.00
G+aa	2.40	-1.43	3.83	3.03	0.13	36.9	168.7	168.7	1	0.26	0.57	0.24	0.56
G-ap+	5.45	-1.62	7.08	6.73	4.54	-73.7	151.6	58.2	2	0.22	0.20	0.20	0.19
Tas	5.66	-1.38	7.04	7.27	3.01	-179.9	-178.0	14.0	2	-0.07	-0.17	-0.07	-0.16
G+ss	7.50	-0.85	8.35	7.66	1.51	-85.6	132.7	132.7	1	0.01	-0.36	0.01	-0.36
G-p+p+	6.42	-3.16	9.59	8.18	0.97	45.2	-5.9	-5.9	1	0.24	0.38	0.22	0.38
G+as	9.28	-2.30	11.57	10.66	6.67	44.5	163.5	-14.2	2	-0.34	-0.26	-0.31	-0.23
G+p+p-	9.10	-2.60	11.70	10.74	5.11	90.1	51.1	-131.0	2	0.19	-0.07	0.18	-0.09
G+as	9.01	-2.64	11.64	10.75	6.26	55.7	-161.7	11.2	2	-0.32	-0.44	-0.29	-0.42

^{S} means calculated with scaled frequencies. Absolute energies (in Hartrees): MP2: -614.3912072817; Cor: -1.705713508; 6-311++G**: -612.685493774; 6-31G*: -612.497420933; ZPE: 0.124831; TCG: 0.088714; ZPE^S 0.114033; TCG^S 0.077249; and T 298.15 K; p 1 atm.

Table S3. Selected energetical and geometrical parameters for conformers of (S,S)-2,3-dideoxy-2,3-difluorotartaric acid dimethyl diester FME.

Conform	MP2	Cor	6-311	6-31	μ	CCCC	FCCO	FCCO	ω	ZPE	TCG	ZPE^s	TCG^s
Tas	0.00	0.00	0.00	0.00	3.00	175.2	-179.9	-2.4	2	0.00	0.00	0.00	0.00
Tss	0.02	-0.44	0.46	0.53	5.26	168.8	-1.8	-1.8	1	-0.04	0.08	-0.04	0.08
Taa	0.02	0.41	-0.39	-0.51	0.57	-178.5	175.9	175.9	1	0.04	-0.07	0.04	-0.07
G-ss	0.50	-2.37	2.86	2.96	4.92	-57.1	26.6	26.6	1	-0.02	0.11	-0.02	0.11
G-as	0.52	-1.90	2.42	2.44	4.70	-54.7	-148.9	27.1	2	-0.03	-0.17	-0.02	-0.17
G-aa	0.90	-1.28	2.17	2.25	1.93	-50.8	-145.5	-145.5	1	-0.01	-0.42	-0.01	-0.42
G-p+p+	1.36	0.10	1.25	1.26	2.61	-67.4	108.3	108.3	1	0.04	-0.45	0.04	-0.46
G+ss	1.59	-1.68	3.27	2.65	0.39	50.0	22.9	22.9	1	0.01	-0.09	0.01	-0.09
G+ss	1.92	-1.78	3.70	3.51	1.66	36.1	-19.7	-19.7	1	-0.13	0.04	-0.12	0.05
G-ap-	1.93	-0.61	2.54	2.44	3.80	-59.9	147.7	-102.1	2	-0.02	-0.16	-0.02	-0.16
G+as	2.10	-1.75	3.84	3.08	3.30	57.8	-143.9	21.6	2	0.01	-0.12	0.01	-0.12
G-p-p-	2.26	-1.70	3.95	4.73	3.85	-54.4	-83.7	-83.7	1	-0.05	-0.62	-0.05	-0.62
G+aa	2.57	-0.53	3.11	2.29	0.78	44.3	153.5	153.5	1	-0.04	-0.03	-0.04	-0.03
G+p+s	2.61	-1.08	3.69	3.09	3.58	41.9	137.6	-20.5	2	-0.06	0.10	-0.05	0.11
G+aa	2.65	-1.86	4.51	3.61	2.49	61.4	-148.2	-148.2	1	0.03	0.01	0.03	0.01

^{S} means calculated with scaled frequencies. Absolute energies (in Hartrees): MP2: -732.4458156367; Cor: -2.036069166; 6-311++G**: -730.409746470; 6-31G*: -730.200599307; ZPE: 0.159610; TCG: 0.119291; ZPE^S 0.145803; TCG^S 0.104592; and T: 298.15 K; p: 1 atm.

Table S4. Selected energetical and geometrical parameters for conformers of (S,S)-2,3-dideoxy-2,3-difluorotartaric acid N,N,N',N'-tetramethyldiamide FTMA

Conform	MP2	Cor	6-311	6-31	μ	CCCC	FCCO	FCCO	ω	ZPE	TCG	ZPE^s	TCG^s
G-aa	0.00	0.00	0.00	0.00	0.92	-28.9	-145.8	-145.8	1	0.00	0.00	0.00	0.00
G-p+p+	0.54	3.57	-3.03	-3.28	1.06	-70.3	107.7	107.7	1	-0.25	-1.01	-0.23	-1.00
Taa	1.96	3.10	-1.14	-1.88	5.07	-171.4	-162.1	-162.1	1	-0.20	-0.67	-0.18	-0.67
G+ss	2.13	-1.10	3.22	2.64	0.56	24.2	27.9	27.9	1	-0.04	0.00	-0.04	0.00
Taa	2.63	3.69	-1.06	-1.66	3.91	-171.6	145.7	-164.3	2	-0.29	-0.94	-0.27	-0.93
Taa	3.15	4.31	-1.15	-1.43	0.66	-170.4	145.0	145.1	1	-0.39	-1.17	-0.36	-1.15
Tas	3.48	2.40	1.08	0.91	2.41	-177.1	14.7	-159.9	2	-0.17	-0.89	-0.16	-0.88
G+p+a	4.50	2.31	2.19	1.06	2.41	45.4	139.8	177.9	2	-0.25	-0.69	-0.23	-0.67
G+aa	5.36	2.62	2.74	1.35	0.92	48.5	148.3	148.4	1	-0.41	-1.01	-0.38	-0.98
G-p+p-	7.15	1.99	5.16	4.67	5.82	-61.3	128.8	-111.8	2	-0.37	-1.05	-0.34	-1.03
G+p+s	8.22	1.11	7.12	6.78	5.31	17.8	101.6	13.8	2	-0.30	-1.15	-0.27	-1.13

^{S} means calculated with scaled frequencies. Absolute energies (in Hartrees): MP2: -771.1273652898; Cor: -2.323859681; 6-311++G**: -768.803505609; 6-31G*: -768.590116073; ZPE: 0.246597; TCG: 0.203269; ZPE^S 0.225267; TCG^S 0.180758; and T 298.15 K; p 1atm.

Table S5. Gibbs free energies and per cents of conformers calculated with scaled and unscaled frequencies as well as with AM1- SM5.4 and PM3-SM5.4 in water and chloroform for (S,S)-2,3-dideoxy-2,3-difluorotartaric acid - FTA.

Conform	G^0_{298K}	%	G^{0S}_{298K}	$\%^S$	ASM-w	$\%^{Aw}$	ASM-c	$\%^{Ac}$	PSM-w	$\%^{Pw}$	PSM-c	$\%^{Pc}$
Tss	0.00	18.3	0.00	18.1	-8.79	44.4	-7.00	30.9	-10.22	47.0	-8.14	34.7
Tas	-0.40	35.7	-0.40	35.7	-8.17	30.4	-6.65	33.4	-9.27	18.4	-7.57	25.9
Taa	0.05	16.9	0.03	17.1	-7.63	5.8	-6.32	9.1	-8.42	2.1	-7.02	4.8
*Tas**	0.42	9.0	0.41	9.0	-8.42	11.7	-6.95	14.0	-10.20	22.3	-8.27	21.3
*Taa**	0.55	7.3	0.53	7.3	-8.02	4.8	-6.71	7.5	-9.50	5.5	-7.82	8.0
G-as	0.81	4.7	0.80	4.7	-6.69	0.3	-5.72	0.9	-7.83	0.2	-6.66	0.7
G-aa	1.17	2.5	1.16	2.5	-6.75	0.2	-5.79	0.6	-7.55	0.1	-6.51	0.3
G-ss	1.65	1.1	1.65	1.1	-6.92	0.1	-5.91	0.3	-8.40	0.1	-7.08	0.4
G-p.+p+	1.43	1.6	1.41	1.7	-6.85	0.1	-5.69	0.3	-7.45	0.0	-6.25	0.1
*Taa***	2.29	0.4	2.27	0.4	-8.82	1.0	-7.39	1.3	-11.00	3.7	-8.92	2.7
G-ap-	1.84	0.8	1.84	0.8	-6.90	0.1	-5.80	0.2	-7.80	0.0	-6.59	0.1
G+ss	2.36	0.3	2.35	0.3	-8.08	0.2	-6.75	0.4	-8.62	0.1	-7.28	0.2
G+aa	2.76	0.2	2.76	0.2	-8.31	0.2	-6.89	0.2	-8.56	0.0	-7.20	0.1
G+as	2.38	0.3	2.38	0.3	-7.50	0.1	-6.38	0.2	-8.09	0.0	-6.93	0.1
G+p+s	2.68	0.2	2.68	0.2	-8.05	0.1	-6.69	0.2	-8.71	0.0	-7.29	0.1
G+ss	2.95	0.1	2.96	0.1	-7.24	0.0	-6.24	0.1	-8.12	0.0	-7.03	0.0
*G-ap+**	2.87	0.1	2.86	0.1	-8.30	0.2	-6.91	0.2	-9.50	0.1	-7.83	0.2
*G-ap-**	3.12	0.1	3.11	0.1	-8.16	0.1	-6.85	0.1	-9.48	0.1	-7.86	0.1
G+aa	3.50	0.0	3.49	0.1	-7.20	0.0	-6.25	0.0	-7.81	0.0	-6.81	0.0
G-p-p-	2.93	0.1	2.92	0.1	-6.24	0.0	-5.39	0.0	-7.50	0.0	-6.42	0.0
*G+aa**	3.54	0.0	3.54	0.0	-8.73	0.1	-7.28	0.1	-9.77	0.1	-8.08	0.1
*G+as**	4.11	0.0	4.11	0.0	-8.85	0.0	-7.34	0.1	-10.36	0.1	-8.46	0.1
*G+aa***	5.33	0.0	5.33	0.0	-9.62	0.0	-8.07	0.0	-11.21	0.0	-9.20	0.0

Table S6. Gibbs free energies and per cents of conformers calculated with scaled and unscaled frequencies as well as with AM1- SM5.4 and PM3-SM5.4 in water and chloroform for (S,S)-2,3-dideoxy-2,3-difluorotartaric acid diamide FAM.

Conform	G^0_{298K}	%	G^{0S}_{298K}	$\%^S$	ASM-w	$\%^{Aw}$	ASM-c	$\%^{Ac}$	PSM-w	$\%^{Pw}$	PSM-c	$\%^{Pc}$
Taa	0.00	99.3	0.00	99.3	-11.02	99.1	-8.54	99.1	-16.55	99.5	-12.67	99.7
G+aa	2.97	0.7	2.96	0.7	-10.81	0.5	-8.61	0.7	-14.41	0.0	-11.47	0.1
G-ap+	5.25	0.0	5.23	0.0	-11.13	0.0	-8.78	0.0	-15.93	0.0	-12.43	0.0
Tas	5.08	0.0	5.09	0.0	-12.84	0.4	-9.84	0.2	-18.48	0.5	-14.13	0.2
G+ss	7.13	0.0	7.13	0.0	-11.24	0.0	-8.86	0.0	-16.11	0.0	-12.57	0.0
G-p+p+	6.81	0.0	6.80	0.0	-9.79	0.0	-7.78	0.0	-13.71	0.0	-10.86	0.0
G+as	8.61	0.0	8.63	0.0	-11.77	0.0	-9.04	0.0	-19.69	0.0	-14.80	0.0
G+p+p-	8.62	0.0	8.60	0.0	-11.41	0.0	-8.94	0.0	-15.85	0.0	-12.32	0.0
G+as	8.16	0.0	8.18	0.0	-11.64	0.0	-8.97	0.0	-19.36	0.0	-14.58	0.0

Table S7. Gibbs free energies and per cents of conformers calculated with scaled and unscaled frequencies as well as with AM1- SM5.4 and PM3-SM5.4 in water and chloroform for (S,S)-2,3-dideoxy-2,3-difluorotartaric acid dimethyl diester FME.

Conform	G^0_{298K}	%	G^{0S}_{298K}	%^{S}	ASM-w	%^{Aw}	ASM-c	%^{Ac}	PSM-w	%^{Pw}	PSM-c	%^{Pc}
Tas	-0.41	30.9	-0.41	30.9	-2.52	28.7	-6.38	35.7	-3.09	20.5	-6.66	31.1
Tss	0.09	13.2	0.10	13.1	-3.39	53.1	-6.95	39.8	-4.34	72.2	-7.50	54.7
Taa	-0.05	16.7	-0.05	16.8	-1.85	5.0	-5.91	8.8	-2.09	2.1	-5.96	5.2
G-*ss*	0.60	5.6	0.60	5.6	-1.75	1.4	-5.50	1.5	-2.40	1.2	-5.84	1.4
G-*as*	-0.07	17.3	-0.06	17.2	-1.44	2.6	-5.41	3.9	-1.87	1.5	-5.60	2.9
G-*aa*	0.48	6.9	0.47	6.9	-1.29	0.8	-5.42	1.6	-1.38	0.3	-5.37	0.8
G-*p*+*p*+	0.91	3.3	0.90	3.4	-1.36	0.4	-5.56	1.0	-1.34	0.1	-5.41	0.4
G+*ss*	1.51	1.2	1.51	1.2	-3.23	3.7	-6.83	3.0	-3.23	1.0	-6.71	1.3
G+*ss*	1.96	0.6	1.97	0.6	-2.47	0.5	-6.39	0.7	-2.62	0.2	-6.37	0.4
G-*ap*-	1.35	1.6	1.36	1.6	-1.59	0.3	-5.72	0.6	-1.85	0.1	-5.79	0.4
G+*as*	1.56	1.1	1.56	1.1	-2.78	1.6	-6.49	1.5	-2.76	0.4	-6.33	0.6
G-*p*-*p*-	1.64	1.0	1.64	1.0	-1.11	0.1	-5.48	0.2	-1.53	0.0	-5.63	0.2
G+*aa*	2.54	0.2	2.55	0.2	-3.24	0.7	-6.95	0.6	-2.90	0.1	-6.58	0.2
G+*p*+*s*	2.30	0.3	2.31	0.3	-3.20	0.9	-6.96	1.0	-3.25	0.3	-6.85	0.4
G+*aa*	2.66	0.2	2.66	0.2	-2.48	0.1	-6.22	0.2	-2.34	0.03	-5.98	0.1

Table S8. Gibbs free energies and per cents of conformers calculated with scaled and unscaled frequencies as well as with AM1- SM5.4 and PM3-SM5.4 in water and chloroform for (S,S)-2,3-dideoxy-2,3-difluorotartaric acid N,N,N',N'-tetramethyldiamide FTMA

Conform	G^0_{298K}	%	G^{0S}_{298K}	%^{S}	ASM-w	%^{Aw}	ASM-c	%^{Ac}	PSM-w	%^{Pw}	PSM-c	%^{Pc}
G-*aa*	0.00	28.5	0.00	28.7	-8.69	7.7	-4.73	18.0	-3.92	20.0	-7.96	11.3
G-*p*+*p*+	-0.46	62.4	-0.46	62.3	-9.65	84.9	-5.06	68.7	-3.89	41.6	-8.59	71.9
Taa	1.29	3.2	1.30	3.2	-9.06	1.6	-4.93	2.8	-4.63	7.5	-8.59	3.7
G+*ss*	2.12	0.8	2.13	0.8	-9.33	0.6	-5.94	3.8	-5.94	16.8	-9.22	2.6
Taa	1.28	3.3	1.29	3.3	-9.33	2.6	-4.99	3.2	-4.53	6.5	-8.78	5.2
Taa	1.98	1.0	2.00	1.0	-9.64	1.3	-5.23	1.5	-4.40	1.6	-8.86	1.8
Tas	2.18	0.7	2.18	0.7	-9.57	0.9	-5.43	1.5	-5.37	5.8	-9.35	3.0
G+*p*+*a*	3.40	0.1	3.42	0.1	-10.04	0.2	-5.57	0.2	-4.53	0.2	-9.12	0.3
G+*aa*	4.35	0.0	4.38	0.0	-10.78	0.2	-6.40	0.2	-4.99	0.1	-9.58	0.1
G-*p*+*p*-	5.69	0.0	5.71	0.0	-9.21	0.0	-4.75	0.0	-4.80	0.0	-9.01	0.0
G+*p*+*s*	6.66	0.0	6.68	0.0	-9.83	0.0	-5.96	0.0	-6.27	0.0	-9.89	0.0