Supporting Information

Quantitative Prediction of the Transformation Potential of Polyfluoroalkyl Substances: A Computational and Machine Learning Study of •OH- Initiated Initial Reaction Kinetics

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Table S1. The dataset for training and test of machine learning. The unit of Δ*E* is used in kcal/mol.

SMILES	Δ*E*	SMILES	Δ*E*	SMILES	Δ*E*	SMILES	Δ*E*
C(C(C(C(CC(C(C(F)(F)OP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	17.53	C(C(C(C(C(C(C(COP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	6.74	C(CC(C(C(C(C(C(C(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	17.56	C(C(C(CC(C(C(C(F)(F)OP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	17.44
C(C(C(C(C(C(C(C(C(COP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	7.17	C(C(C(C(C(C(C(C(COP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	6.49	C(C(C(C(C(C(C(C(CS(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	14.42	C(C(C(C(C(C(C(C(C(CS(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	14.64
C(C(C(CO)(F)F)(F)F)(F)(F)F	12.62	C(C(CO)(F)F)(F)(F)F	12.43	C(CS(=O)(=O)[O-])(F)(F)F	15.28	C(C(C(C(CO)(F)F)(F)F)(F)F)(F)(F)F	13.33
C(C(C(C(C(CCCS(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)(F)F	10.80	C(C(C(C(C(C(CC(F)(F)OP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	14.84	C(C(C(C(C(CC(C(F)(F)OP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)(F)F	17.33	C(C(C(C(C(C(CCC(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	9.96
C(C(CO)(C(F)(F)F)F)(F)(F)F	12.14	C(C(CS(=O)(=O)[O-])(F)F)(F)(F)F	15.49	C(CO)(F)(F)F	12.41	C(C(CO)C(F)(F)F)(F)(F)F	10.36
C(C(C(C(C(C(CO)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	12.61	C(C(C(CS(=O)(=O)[O-])(F)F)(F)F)(F)(F)F	15.53	C(C(C(C(CCCCOP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)(F)F	5.24	C(C(C(C(C(CO)(F)F)(F)F)(F)F)(F)F)(F)(F)F	12.75
C(C(C(C(C(C(C(CO)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	12.67	C(C(C(C(C(C(C(C(CO)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	11.29	C(C(CC(C(C(C(C(F)(F)OP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)(F)F	17.06	C(CC(C(C(C(C(C(F)(F)OP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	17.16
C(C(C(C(CS(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)(F)F	14.95	C(C(C(C(C(CS(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)(F)F	14.68	C(C(CO)(C(F)(F)F)C(F)(F)F)(F)(F)F	12.05	C(C(C(CO)(F)F)C(F)(F)F)(F)(F)F	12.48
C(C(C(C(C(C(C(C(C(CO)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	12.49	C(C(C(C(C(C(CS(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	15.08	CC(C(C(C(C(C(C(F)(F)OP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	16.96	C(C(C(C(CC(C(C(F)(F)S(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	17.16
C(CC(=O)[O-])(F)(F)F	12.28	C(C(CC(=O)[O-])(F)F)(F)(F)F	13.69	C(C(CC(=O)[O-])(C(F)(F)F)F)(F)(F)F	12.43	C(C(CC(=O)[O-])C(F)(F)F)(F)(F)F	11.23
C(C(C(C(C(C(C(CS(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	14.75	CC(C(C(C(C(C(C(C(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	15.01	C(C(C(C(C(CC(C(F)(F)S(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)(F)F	16.72	C(C(C(C(C(C(CC(F)(F)S(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	16.00
C(C(C(C(CCCCS(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)(F)F	8.92	C(C(C(C(C(C(CCO)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	9.28	C(C([C@@](CO)(F)C(F)(F)F)C(F)(F)F)(F)(F)F	12.29	C(C(CC(=O)[O-])(C(F)(F)F)C(F)(F)F)(F)(F)F	13.92
C(C(C(C(C(CC(C(O)(F)	17.90	C(C(C(C(C(C(CC(O)(F)	17.13	C(C(C(CC(C(C(C(F)(F)S(	16.35	C(C(CC(C(C(C(C(F)	17.28

F)(F)F)(F)F)(F)F)(F)F)(F)(F)F		F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F		=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F		(F)S(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)(F)F	
C(C(C(C(C(C(CC(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)(F)F	14.00	C(C(C(C(CC(=O)[O-])(F)F)(F)F)(F)F)(F)(F)F	12.62	C(C(C(CC(=O)[O-])(F)F)C(F)(F)F)(F)(F)F	11.60	C(C([C@@](CC(=O)[O-])(F)C(F)(F)F)C(F)(F)F)(F)(F)F	11.70
C(C(C(C(C(C(C(CC(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	11.93	C(C(C(C(CC(C(C(O)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	16.83	C(CC(C(C(C(C(C(F)(F)S(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	17.69	C(C(C(C(C(CC(C(C(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	17.84
C(C(C(C(C(C(C(CC(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	13.05	C(C(C(CC(C(C(C(O)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	17.46	CC(C(C(C(C(C(C(S(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	15.39	C(C(C(C(C(C(C(C(CC(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	11.71
C(C(COP(=O)([O-])[O-])(C(F)(F)F)F)(F)(F)F	6.70	C(C(CC(C(C(C(C(O)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	17.59	C(C(C(COP(=O)([O-])[O-])(F)F)C(F)(F)F)(F)(F)F	6.77	C(C(COP(=O)([O-])[O-])(C(F)(F)F)C(F)(F)F)(F)(F)F	6.17
C(C(C(C(C(C(C(C(C(C(C=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	13.96	C(CC(C(C(C(C(C(O)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	16.97	C(C([C@@](COP(=O)([O-])[O-])(F)C(F)(F)F)C(F)(F)F)(F)(F)F	7.35	C(C(C(C(C(C(CCS(=O)(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	13.03
C(C([C@@](CS(=O)(=O)[O-])(F)C(F)(F)F)C(F)(F)F)(F)(F)F	15.62	CC(C(C(C(C(C(C(O)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	16.27	C(C(C(C(CCCCO)(F)F)(F)F)(F)F)(F)F	7.85	C(C(C(C(C(CCCO)(F)F)(F)F)(F)F)(F)F)(F)F	8.76
C(C(COP(=O)([O-])[O-])(F)F)(F)(F)F	6.42	C(COP(=O)([O-])[O-])(F)(F)F	7.03	C(C(C(CC(=O)[O-])(F)F)(F)F)(F)(F)F	13.97	C(C(CS(=O)(=O)[O-])C(F)(F)F)(F)(F)F	13.47
C(C(C(COP(=O)([O-])[O-])(F)F)(F)F)(F)(F)F	7.19	C(C(COP(=O)([O-])[O-])C(F)(F)F)(F)(F)F	5.88	C(C(C(C(C(CCCC(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F	10.39	C(C(CS(=O)(=O)[O-])(C(F)(F)F)F)(F)(F)F	14.65
C(C(C(C(COP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)(F)F	7.22	C(C(C(CS(=O)(=O)[O-])(F)F)C(F)(F)F)(F)(F)F	15.45	C(C(C(C(CCCCC(=O)[O-])(F)F)(F)F)(F)F)(F)F	9.29	C(C(CS(=O)(=O)[O-])(C(F)(F)F)C(F)(F)F)(F)(F)F	13.05
C(C(C(C(C(COP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F	6.33	C(C(C(CC(C(C(C(C(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	16.98	C(C(C(C(C(C(CCOP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	9.05	C(C(C(C(CC(C(C(C(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	17.38
C(C(C(C(C(C(COP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	6.64	C(C(CC(C(C(C(C(C(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	17.37	C(C(C(C(C(CCCOP(=O)([O-])[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F	10.03	C(C(C(C(C(C(CC(C(C(=O)[O-])(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)(F)F	13.34

Table S2. Molecular feature matrix of the molecular fingerprints and physicochemical descriptors.

Descriptor Type	Dimensionality	Parameter Settings	Description
Morgan Fingerprints	2048	radius=2, nBits=2048	Circular topology-based molecular fingerprints capturing local chemical environments
MACCS Fingerprints	167	Default parameters (166 MACCS structural keys + 1 identifier bit)	SMARTS pattern-based molecular structural keys
E-state Fingerprints	79	Default parameters	Electrotopological state indices reflecting atomic electronic states and topological environments
RDKit Physicochemical Descriptors	91	Default parameters (including LogP, molecular weight, number of hydrogen bond donors/acceptors, etc.)	Molecular physicochemical properties calculated based on RDKit

Table S3. Hyperparameter searching intervals and finalized optimal parameters of the machine learning models.

Algorithm-Fingerprint	Hyperparameter
Random Forest-E-state	min_samples_leaf=1, max_depth=9, n_estimators=5, max_features=40, min_samples_split=3, random_state=20, bootstrap=True, n_jobs=-1
Random Forest-MACCS	min_samples_leaf=1, max_depth=9, n_estimators=4, max_features=32, min_samples_split=2, random_state=20, bootstrap=True, n_jobs=-1
Random Forest-Morgan	min_samples_leaf=1, max_depth=17, n_estimators=49, max_features=95, min_samples_split=2, random_state=20, bootstrap=True, n_jobs=-1
Random Forest-Descriptor	min_samples_leaf=1, max_depth=9, n_estimators=6, max_features=16, min_samples_split=2, random_state=20, bootstrap=True, n_jobs=-1
XGBoost-E-state	min_child_weight=1, learning_rate=0.5, colsample_bytree=0.6, max_depth=2, n_estimators=9, random_state=1, n_jobs=-1, subsample=0.7
XGBoost-MACCS	min_child_weight=1, learning_rate=0.4, colsample_bytree=0.8, max_depth=2, n_estimators=10, random_state=1, n_jobs=-1, subsample=0.8
XGBoost-Morgan	min_child_weight=1, learning_rate=0.3, colsample_bytree=0.6, max_depth=2, n_estimators=33, random_state=1, n_jobs=-1, subsample=0.8
XGBoost-Descriptor	min_child_weight=1, learning_rate=0.4, colsample_bytree=0.8, max_depth=4, n_estimators=29, random_state=1, n_jobs=-1, subsample=0.8
SVM-E-state	kernel='rbf', C=1, gamma=0.1, epsilon=2
SVM-MACCS	kernel='rbf', C=20, gamma=0.01, epsilon=0.5
SVM-Morgan	kernel='rbf', C=14, gamma=0.001, epsilon=0.01
SVM-Descriptor	kernel='rbf', C=30, gamma=0.01, epsilon=0.5

Table S4. Optimized transition state structures for representative compounds F-$(CF_2)_m$-CH_2-X (X = –OH, $–COO^–$, $–PO_4^{2–}$, $–SO_3^–$; m=1-9), the unit of bond lengths are used in Å.

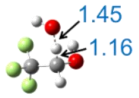
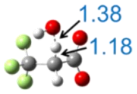
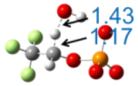
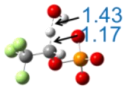
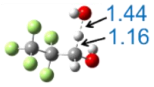
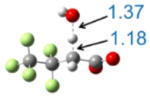
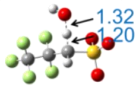
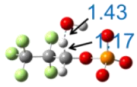
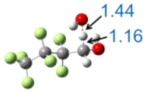
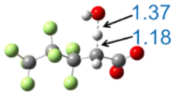
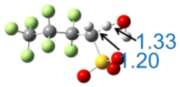
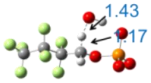
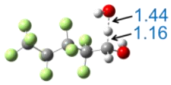
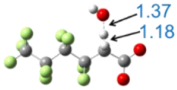
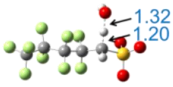
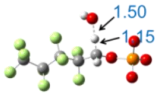
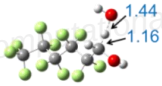
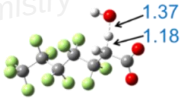
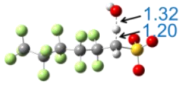
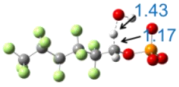
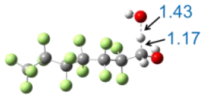
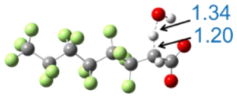
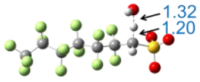
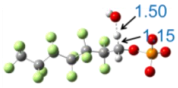
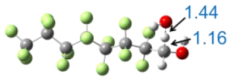
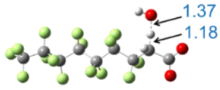
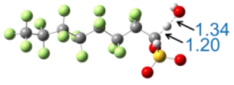
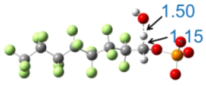
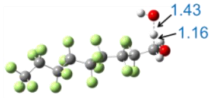
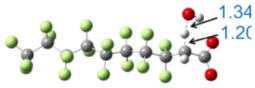
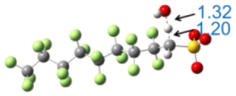
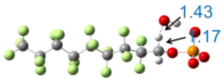
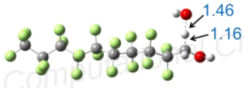
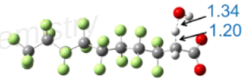
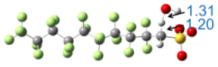
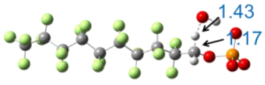
m	Functional group (X)			
	OH	COO^-	SO_3^-	PO_4^{2-}
1				
2				
3				
4				
5				
6				
7				
8				
9				

Table S5. Optimized transition state structures for representative compounds F-$(CF_2)_{7-m}$-(CH_2)-$(CF_2)_m$-X (X = –OH, $–COO^–$, $–PO_4^{2–}$, $–SO_3^–$; m=1-7), the unit of bond lengths are used in Å.

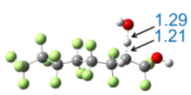
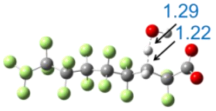
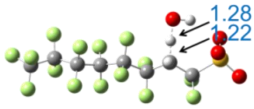
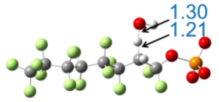
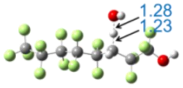
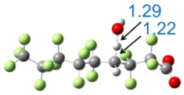
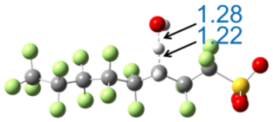
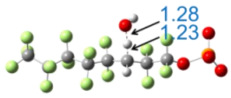
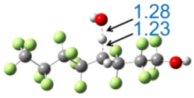
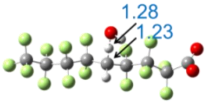
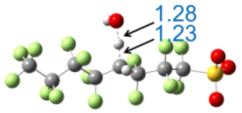
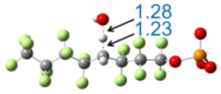
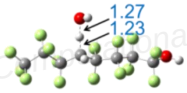
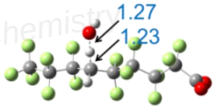
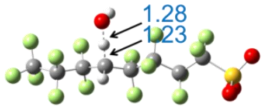
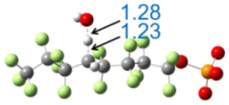
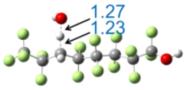
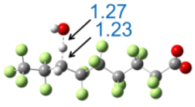
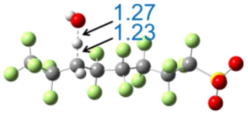
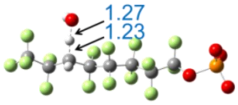
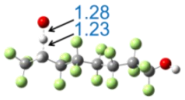
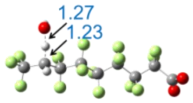
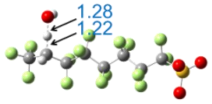
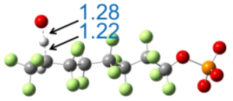
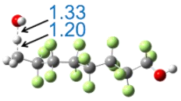
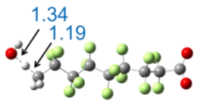
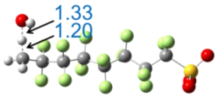
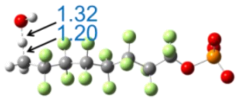
m	Functional group (X)			
	OH	COO^-	SO_3^-	PO_4^{2-}
1				
2				
3				
4				
5				
6				
7				

Table S6. Optimized transition state structures for representative compounds $F–(CF_2)_{8-m}–(CH_2)_m–X$ (X = –OH, $–COO^-$, $–PO_4^{2-}$, $–SO_3^-$; m = 1–4), the unit of bond lengths are used in Å.

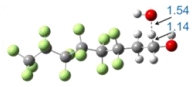
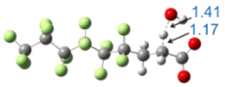
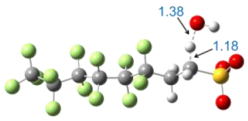
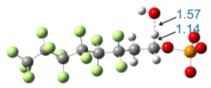
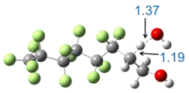
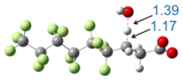
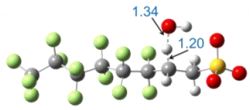
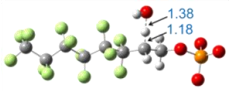
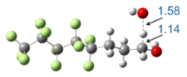
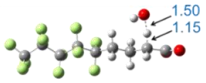
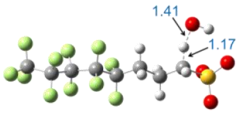
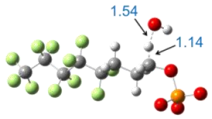
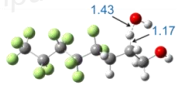
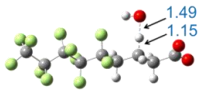
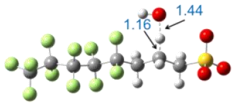
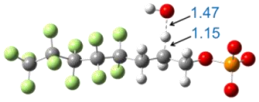
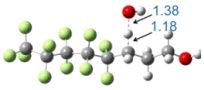
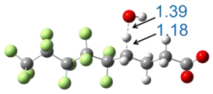
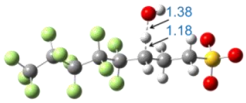
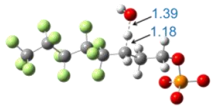
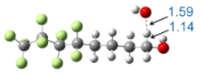
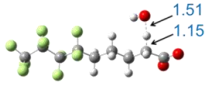
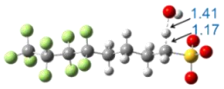
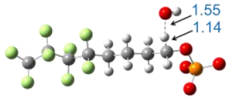
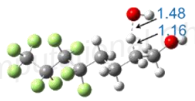
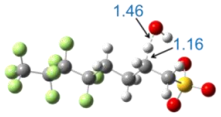
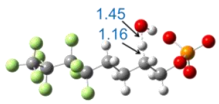
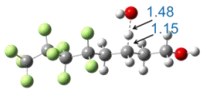
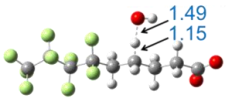
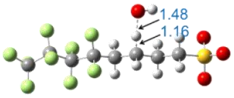
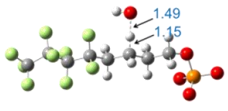
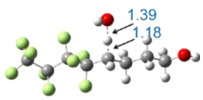
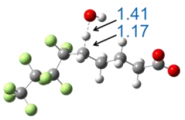
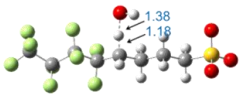
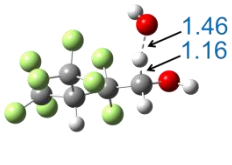
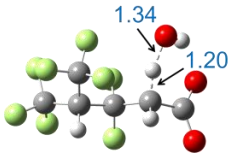
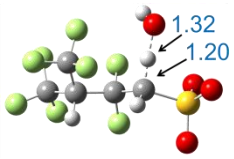
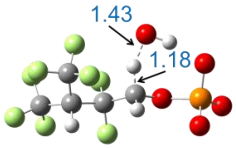
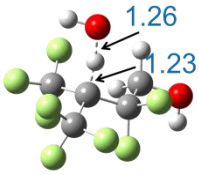
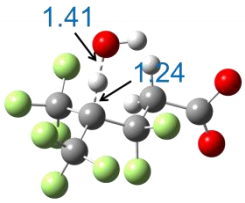
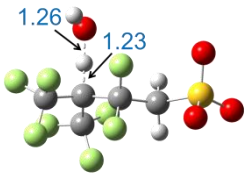
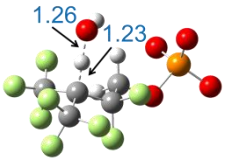
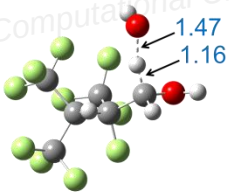
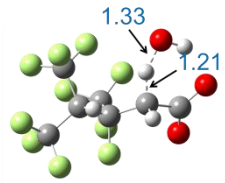
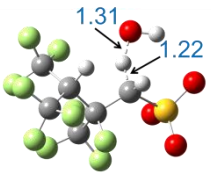
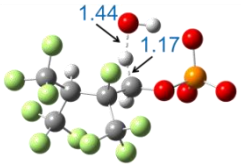
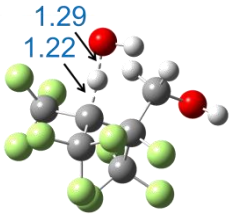
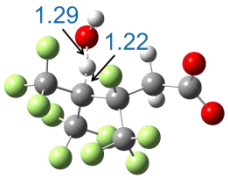
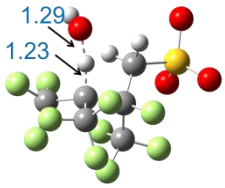
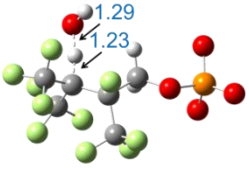
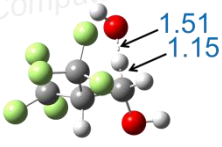
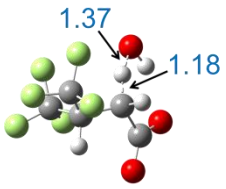
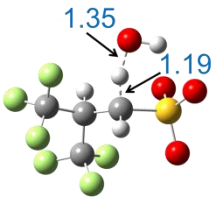
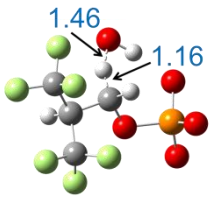
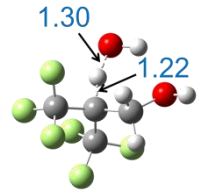
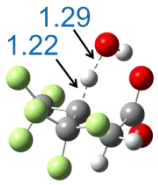
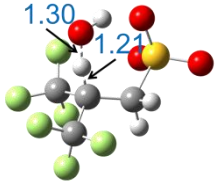
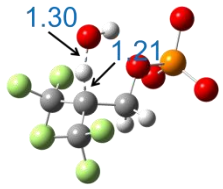
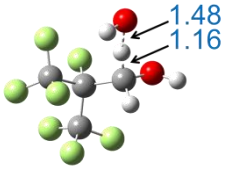
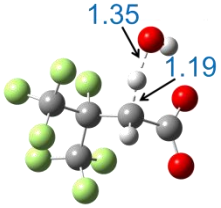
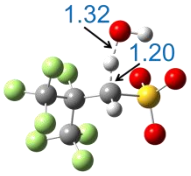
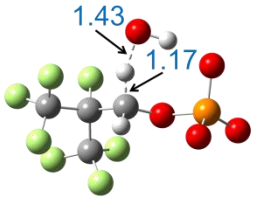
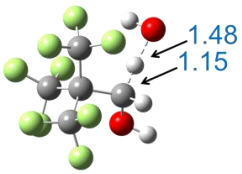
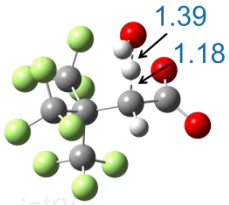
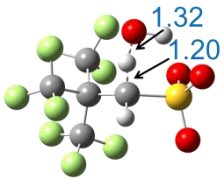
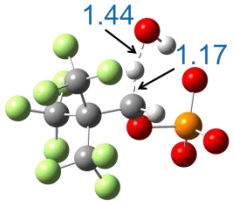
m (site)	Functional group (X)			
	OH	COO^-	SO_3^-	PO_4^{2-}
2(α)				
2(β)				
3(α)				
3(β)				
3(γ)				
4(α)				
4(β)				
4(γ)				
4(δ)				

Table S7. Optimized transition state structures for the branched polyfluoroalkyl compounds (Figure 4), the unit of bond lengths are used in Å.

Name (site)	Functional group (X)			
	OH	COO^-	SO_3^-	PO_4^{2-}
4-1 (α)				
4-1 (γ)				
4-2 (α)				
4-2 (γ)				
4-3 (α)				

4-3 (β)				
4-4				
4-5				

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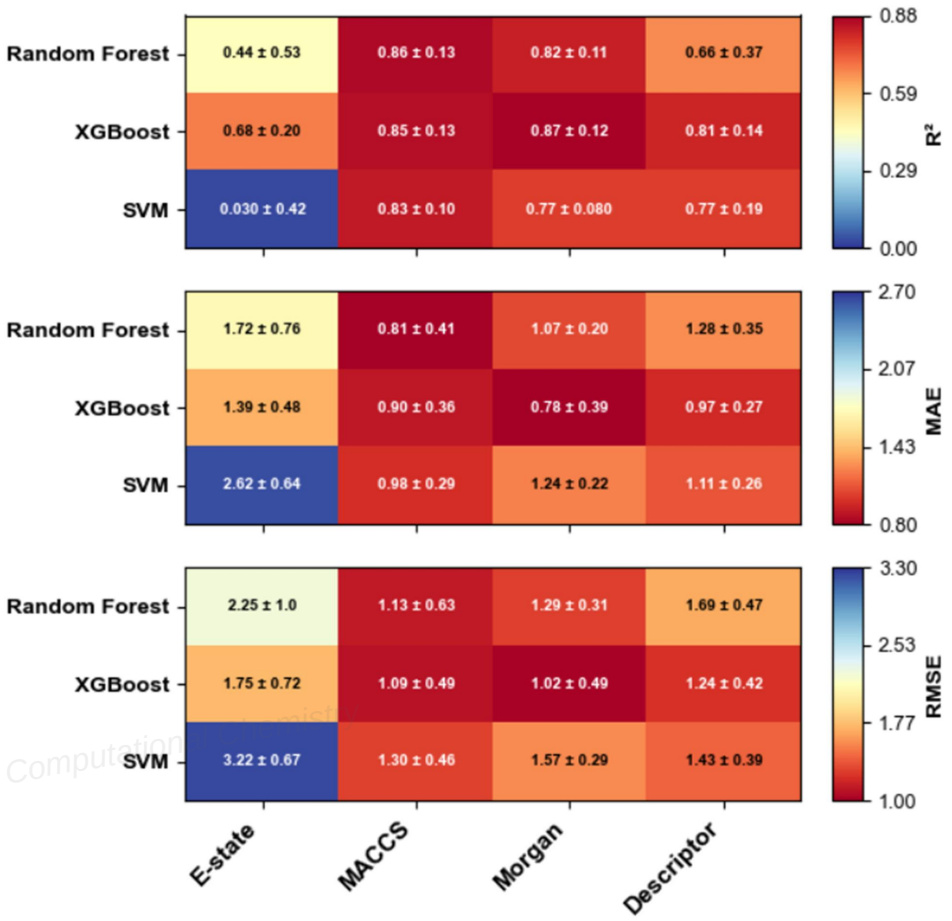
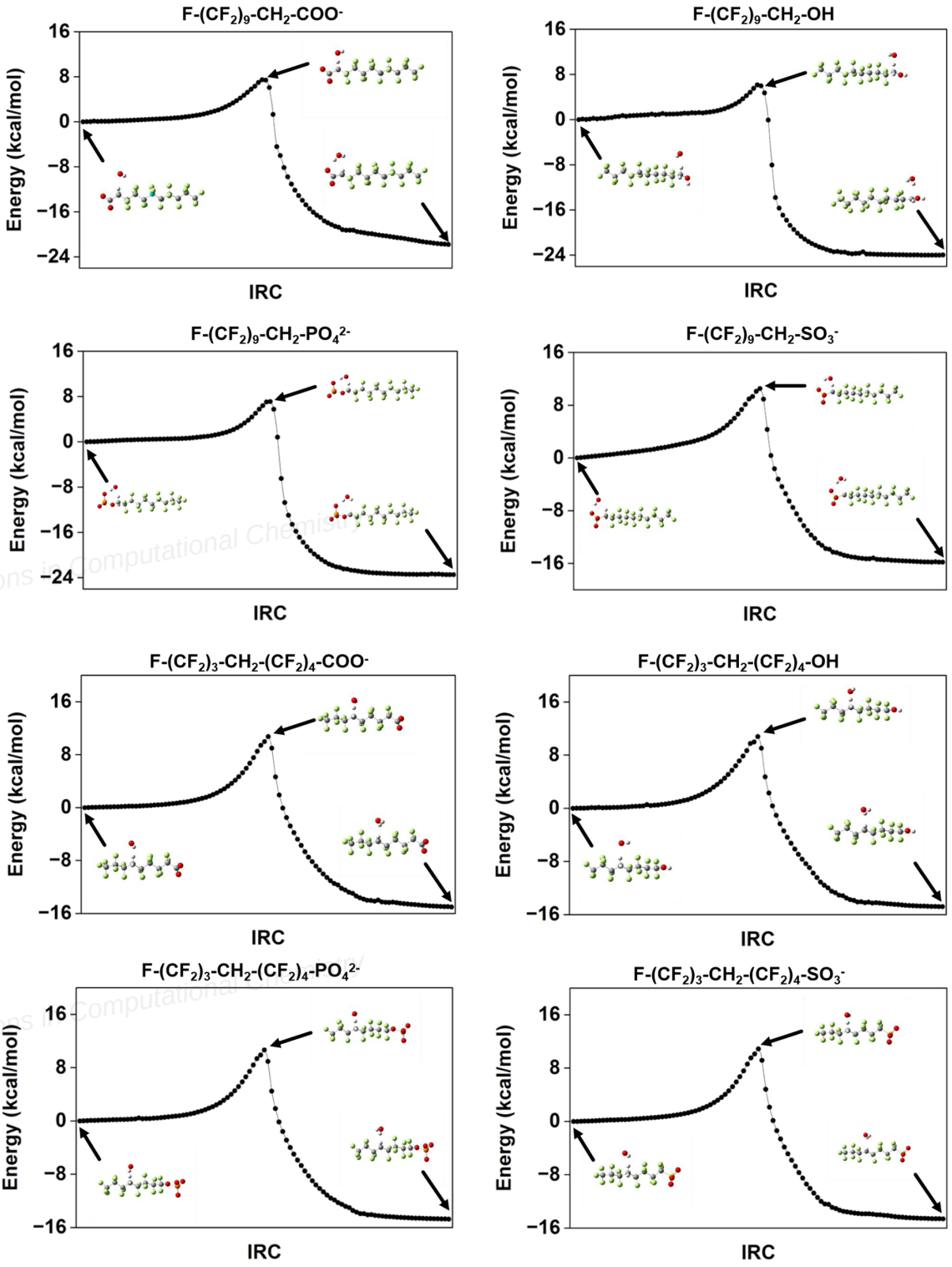
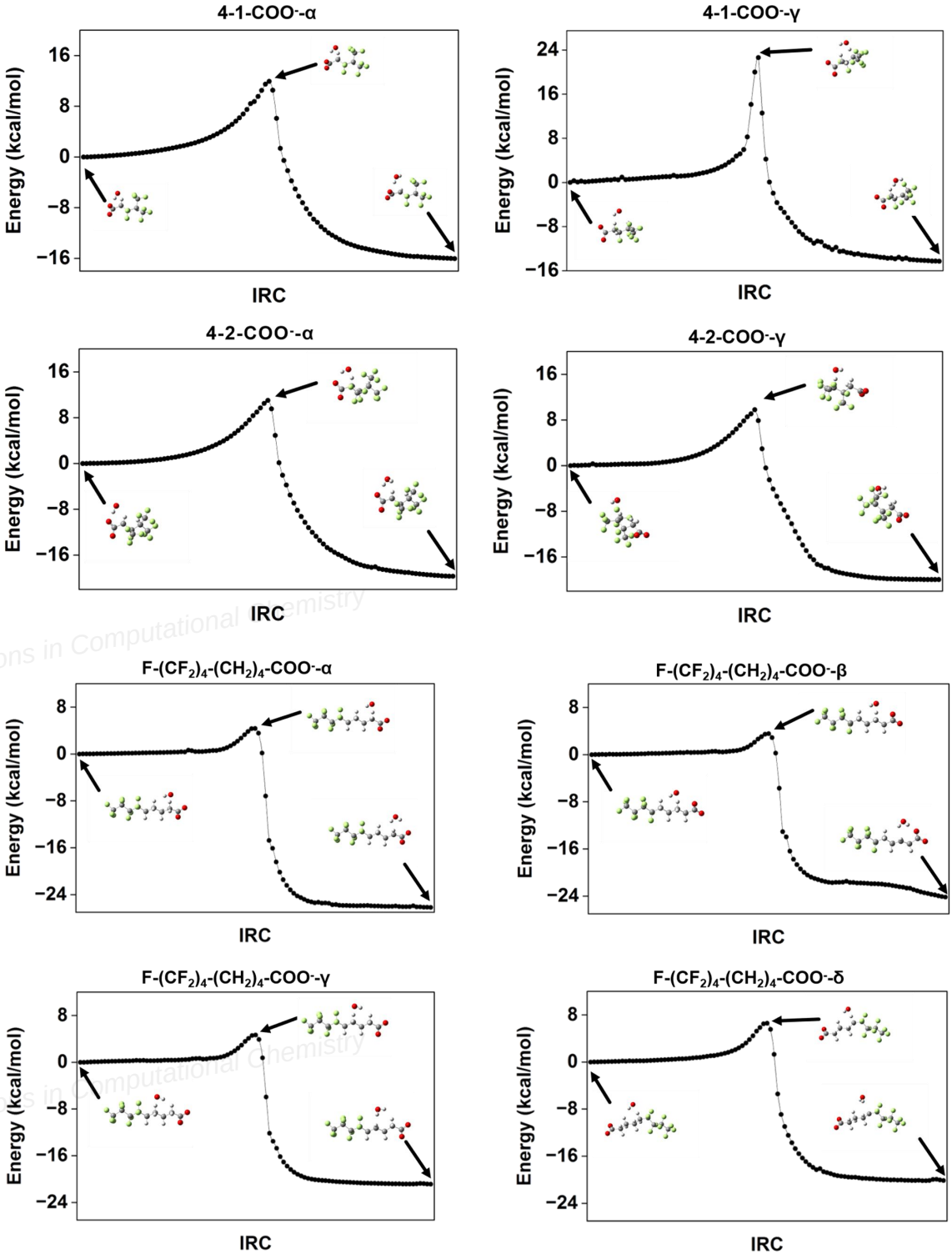


Figure S1. Heatmaps of the predictive performance metrics (R^2, MAE, and RMSE) on the training set of the 12 machine learning models.

IRC of representative transition states





Coordinates of all the transition states involved in this study

(1-1) Formula: F-(CF_2)$_m$-CH_2-OH

m=1

Charge = 0 Multiplicity = 2

C	-0.647294	-0.246048	-0.023954
C	0.409741	0.680171	-0.571961
H	0.298009	0.763325	-1.650458
H	1.428098	0.152637	-0.381736
F	-1.883081	0.216431	-0.247278
F	-0.527645	-0.410499	1.301196
O	0.371014	1.942537	0.002579
H	0.491538	1.876852	0.958527
O	2.600055	-0.610332	-0.018789
H	2.164824	-1.22749	0.594983
F	-0.558797	-1.453454	-0.589046

m=2

Charge = 0 Multiplicity = 2

C	-1.16288	0.345855	0.106707
C	0.005981	-0.616306	-0.138123
C	1.275642	-0.277312	0.61295
H	1.085588	-0.212491	1.681399
H	1.621269	0.772478	0.252148
F	-1.475097	0.377174	1.397473
F	-0.850765	1.575395	-0.286994
F	-0.429363	-1.84882	0.205914
F	0.233429	-0.630723	-1.471174
O	2.276817	-1.21072	0.376771
H	2.482884	-1.244255	-0.566514
O	2.144035	2.036728	-0.194535
H	1.495295	2.601048	0.261248
F	-2.229794	-0.055056	-0.575816

m=3

Charge = 0 Multiplicity = 2

C	-1.848706	-0.021336	-0.010694
C	-0.395508	0.479287	0.108768
C	0.667055	-0.626982	-0.060903

C	2.012373	-0.298045	0.556312
H	1.925663	-0.231934	1.637353
H	2.342471	0.751608	0.175399
F	-2.202294	-0.712657	1.061546
F	-1.97747	-0.787619	-1.086949
F	-0.260813	1.057631	1.312672
F	-0.215505	1.410109	-0.837446
F	0.179325	-1.766399	0.488566
F	0.804018	-0.861629	-1.384319
O	2.964852	-1.253293	0.22588
H	3.054579	-1.308309	-0.734579
O	2.669628	2.104046	-0.20412
H	1.997543	2.545819	0.34362
F	-2.661413	1.020481	-0.127045

m=4

Charge = 0 Multiplicity = 2

C	2.401787	0.337775	0.089081
C	1.157557	-0.562895	-0.074634
C	-0.161572	0.234757	-0.193725
C	-1.41948	-0.613282	0.087435
C	-2.69049	-0.019203	-0.486252
H	-2.642588	-0.003333	-1.571435
H	-2.758759	1.086606	-0.13029
F	2.369898	1.323796	-0.798535
F	2.450419	0.851119	1.307822
F	1.326645	-1.296466	-1.179553
F	1.095496	-1.375771	0.988243
F	-0.237741	0.735616	-1.436687
F	-0.12291	1.257341	0.675767
F	-1.214353	-1.848873	-0.42943
F	-1.53095	-0.7588	1.425432
O	-3.813547	-0.730835	-0.085888
H	-3.876455	-0.733906	0.877887
O	-2.818962	2.494631	0.171479
H	-2.051332	2.763755	-0.363361
F	3.492651	-0.386451	-0.111832

m=5

Charge = 0 Multiplicity = 2

C	-1.71165	0.53449	-0.209777

C	-0.534423	-0.449956	0.000375
C	0.822512	0.275635	0.165053
C	2.042329	-0.636822	-0.086259
C	3.322076	-0.121546	0.542063
H	3.234389	-0.112816	1.624744
H	3.464673	0.980004	0.198951
F	-1.555487	1.602154	0.582858
F	-1.721931	0.932825	-1.484897
F	-0.774621	-1.18364	1.095216
F	-0.473483	-1.26261	-1.062481
F	0.890742	0.765204	1.412616
F	0.859655	1.29934	-0.702363
F	1.753027	-1.867053	0.402126
F	2.194877	-0.767777	-1.421603
O	4.417094	-0.892971	0.176286
H	4.513712	-0.897495	-0.78469
O	3.641964	2.384803	-0.075436
H	2.909742	2.701984	0.481933
C	-3.086828	-0.093012	0.105698
F	-3.251176	-0.222352	1.412102
F	-3.18383	-1.285546	-0.46778
F	-4.039892	0.694004	-0.369199

m=6

Charge = 0 Multiplicity = 2

C	3.722066	-0.053071	-0.140307
C	2.360229	0.363547	0.458537
C	1.156031	-0.099932	-0.397381
C	-0.170318	-0.106425	0.405798
C	-1.417558	-0.066029	-0.511065
C	-2.711755	-0.541157	0.182448
C	-3.970053	-0.110683	-0.549873
H	-3.896896	-0.351172	-1.609124
H	-4.040996	1.049717	-0.474409
F	3.93114	-1.347471	0.034762
F	3.748979	0.222146	-1.437771
F	2.26761	-0.163657	1.685589
F	2.338538	1.696083	0.549058
F	1.392296	-1.337287	-0.850414
F	1.03814	0.728553	-1.442419
F	-0.204207	-1.214217	1.155912

F	-0.192102	0.965491	1.209901
F	-1.194202	-0.850358	-1.577953
F	-1.581111	1.195853	-0.935187
F	-2.661872	-1.886823	0.269183
F	-2.709769	-0.063148	1.451012
O	-5.109813	-0.699687	-0.020083
H	-5.229455	-0.426513	0.898846
F	4.68622	0.622241	0.465251
O	-4.236579	2.429047	-0.142231
H	-3.610294	2.468922	0.60195

m=7

Charge = 0 Multiplicity = 2

C	4.344354	-0.039992	-0.226888
C	3.010832	0.387344	0.424216
C	1.783964	-0.352897	-0.162598
C	0.454535	0.38477	0.137386
C	-0.778677	-0.544391	-0.003415
C	-2.096857	0.245612	-0.188651
C	-3.359629	-0.588379	0.118938
C	-4.615007	-0.042967	-0.533454
H	-4.538529	-0.118237	-1.614485
H	-4.689477	1.088385	-0.271856
F	4.44478	0.44891	-1.451649
F	4.417609	-1.363489	-0.276096
F	2.864553	1.705786	0.24483
F	3.087977	0.125469	1.731579
F	1.928843	-0.458202	-1.488673
F	1.735494	-1.580462	0.369052
F	0.33406	1.407351	-0.717475
F	0.497668	0.861446	1.38759
F	-0.595538	-1.341039	-1.064667
F	-0.870381	-1.29608	1.100634
F	-2.156728	0.67913	-1.456843
F	-2.067712	1.309887	0.62874
F	-3.138768	-1.85724	-0.302387
F	-3.507632	-0.638195	1.459961
O	-5.749551	-0.718303	-0.104332
H	-5.838845	-0.637575	0.853906
F	5.347345	0.423413	0.502135
O	-4.78194	2.5163	-0.105059

H	-4.03645	2.748675	-0.686198

m=8

Charge = 0 Multiplicity = 2

C	4.990661	-0.170523	-0.041682
C	3.651908	0.546515	0.239794
C	2.423803	-0.235821	-0.285445
C	1.101866	0.236269	0.371547
C	-0.144126	-0.179264	-0.452447
C	-1.445975	-0.139682	0.389305
C	-2.717741	-0.078354	-0.494085
C	-4.005528	-0.500213	0.243402
C	-5.274866	-0.107743	-0.490663
H	-5.23299	-0.438025	-1.526923
H	-5.331844	1.054085	-0.513173
F	5.13674	-1.214975	0.756523
F	5.028427	-0.575402	-1.304274
F	3.539239	0.714238	1.563003
F	3.690361	1.740891	-0.35591
F	2.594157	-1.538106	-0.030563
F	2.340815	-0.057366	-1.60939
F	1.015803	-0.297084	1.595578
F	1.124436	1.57041	0.475254
F	0.036424	-1.423277	-0.912602
F	-0.267283	0.657558	-1.489541
F	-1.488032	-1.232562	1.159669
F	-1.414315	0.945553	1.175265
F	-2.548142	-0.888232	-1.55177
F	-2.853473	1.180328	-0.937401
F	-3.966364	-1.839729	0.405883
F	-3.978204	0.052182	1.48042
O	-6.408013	-0.632211	0.116451
H	-6.501086	-0.274863	1.009189
F	5.986397	0.674834	0.171462
O	-5.516528	2.460586	-0.306926
H	-4.810624	2.581353	0.351923

m=9

Charge = 0 Multiplicity = 2

C	-5.598882	0.398581	-0.005406
C	-4.322447	-0.471114	0.007985
C	-3.028188	0.354362	-0.196702

C	-1.766799	-0.406394	0.284802
C	-0.465431	0.161878	-0.337356
C	0.796587	-0.248264	0.466119
C	2.092485	-0.123985	-0.374524
C	3.367615	-0.068442	0.504714
C	4.656497	-0.421585	-0.268214
C	5.916603	0.014154	0.444089
H	5.912205	-0.325861	1.480423
H	5.918882	1.17055	0.479122
F	-5.562649	1.237303	-1.032816
F	-5.702754	1.089505	1.11785
F	-6.656764	-0.387185	-0.125848
F	-4.420681	-1.367974	-0.975966
F	-4.264757	-1.109409	1.183228
F	-2.902909	0.629735	-1.500427
F	-3.126084	1.502277	0.483684
F	-1.882142	-1.694683	-0.05793
F	-1.692339	-0.310597	1.617446
F	-0.355461	-0.293791	-1.59059
F	-0.544583	1.497722	-0.361791
F	0.662219	-1.518	0.867692
F	0.893532	0.543667	1.540499
F	2.165176	-1.17489	-1.199615
F	2.022116	0.998989	-1.102735
F	3.229305	-0.932146	1.523634
F	3.473746	1.169745	1.008577
F	4.66492	-1.758551	-0.454775
F	4.581861	0.149916	-1.493682
O	6.998952	-0.448169	-0.295535
H	7.768325	-0.503929	0.281838
O	5.998246	2.621141	0.291659
H	5.299002	2.695631	-0.38131

(1-2) Formula: $F-(CF_2)_m-CH_2-COO^-$

m=1

Charge = -1 Multiplicity = 2

C	0.871022	-0.519469	0.038266
C	-0.200888	0.229273	-0.689789
H	-0.139449	0.003823	-1.751082
H	0.051571	1.371306	-0.550286
C	-1.594932	-0.021989	-0.096279
F	0.919422	-0.210942	1.342651
F	0.695025	-1.849627	-0.034409
O	-1.962431	0.720378	0.836955
O	-2.225131	-0.973789	-0.606821
O	0.544727	2.621541	-0.254063
H	1.438822	2.500088	-0.617677
F	2.090056	-0.266893	-0.464098

m=2

Charge = -1 Multiplicity = 2

C	-1.668288	0.075688	0.21469
C	-0.286146	-0.472488	-0.172514
C	0.855219	0.209851	0.520729
H	0.670743	0.294602	1.589946
H	0.891304	1.332885	0.144319
C	2.256685	-0.336895	0.226398
F	-1.762382	1.369881	-0.072679
F	-1.886679	-0.086677	1.516121
F	-0.208194	-0.365959	-1.519371
F	-0.326121	-1.795222	0.127098
O	3.172528	0.185032	0.901421
O	2.371032	-1.22197	-0.64644
O	0.98256	2.562435	-0.452493
H	0.528357	2.343744	-1.285335
F	-2.621533	-0.57004	-0.451686

m=3

Charge = -1 Multiplicity = 2

C	2.252334	-0.236866	-0.018581
C	0.903363	0.506463	-0.114007
C	-0.336562	-0.400272	0.069515

C	-1.604416	0.203508	-0.458314
H	-1.517604	0.394771	-1.525746
H	-1.741513	1.266168	0.039867
C	-2.902895	-0.557014	-0.14972
F	2.268963	-1.040342	1.037495
F	2.474911	-0.953188	-1.110777
F	0.897028	1.454647	0.834432
F	0.865076	1.105904	-1.314915
F	-0.415087	-0.66927	1.392628
F	-0.058813	-1.571749	-0.562083
O	-2.803463	-1.719827	0.291922
O	-3.95337	0.073117	-0.400393
O	-1.851494	2.588177	0.386631
H	-1.132018	2.933723	-0.169831
F	3.233121	0.64941	0.10734

m=4

Charge = -1 Multiplicity = 2

C	2.847049	0.227844	0.096783
C	1.545437	-0.575993	-0.111903
C	0.283631	0.317088	-0.193232
C	-1.036388	-0.450541	0.065488
C	-2.254264	0.262001	-0.445465
H	-2.17836	0.426686	-1.517894
H	-2.279756	1.340944	0.036752
C	-3.611493	-0.362765	-0.088514
F	2.922173	0.685981	1.336246
F	2.89351	1.249019	-0.749571
F	1.435442	-1.440043	0.905343
F	1.671577	-1.260287	-1.254794
F	0.402213	1.304994	0.710448
F	0.254043	0.869071	-1.416655
F	-1.098236	-0.66541	1.398456
F	-0.900023	-1.662251	-0.535392
O	-3.61243	-1.504568	0.414179
O	-4.603024	0.347026	-0.36531
O	-2.264	2.670874	0.372169
H	-1.557077	2.958624	-0.231462
F	3.886744	-0.563153	-0.12682

m=5

Charge = -1 Multiplicity = 2

C	-3.487092	-0.212966	0.110214
C	-2.149396	0.488312	-0.216018
C	-0.915941	-0.414656	0.030854
C	0.396936	0.397214	0.163975
C	1.674505	-0.445452	-0.073101
C	2.917654	0.183713	0.484412
H	2.8293	0.312071	1.561049
H	3.008651	1.276526	0.044723
C	4.244462	-0.504548	0.128424
F	-3.503119	-1.43123	-0.414858
F	-3.66003	-0.300857	1.419064
F	-2.175326	0.847154	-1.502817
F	-2.064156	1.586951	0.545231
F	-0.816888	-1.2716	-0.993087
F	-1.115274	-1.110493	1.159579
F	0.363928	1.402502	-0.727978
F	0.42918	0.924373	1.397561
F	1.763512	-0.639698	-1.407685
F	1.447322	-1.656624	0.500917
O	4.18969	-1.651468	-0.360152
O	5.269542	0.160181	0.393903
O	3.053684	2.613932	-0.257777
H	2.297065	2.90475	0.280632
F	-4.48305	0.491277	-0.405564

m=6

Charge = -1 Multiplicity = 2

C	-4.083498	0.302729	-0.31064
C	-2.839132	-0.445974	0.214891
C	-1.528669	0.359215	0.029087
C	-0.270187	-0.542517	0.08695
C	1.023016	0.263518	0.371025
C	2.319198	-0.471133	-0.03846
C	3.554651	0.144918	0.553382
H	3.58714	-0.009385	1.630222
H	3.463241	1.329409	0.407417
C	4.857839	-0.306425	-0.125692
F	-4.111066	0.288022	-1.633167

F	-4.0653	1.559736	0.113377
F	-2.749774	-1.611286	-0.437816
F	-3.018689	-0.684575	1.516538
F	-1.563276	0.981565	-1.156107
F	-1.45925	1.278985	0.999715
F	-0.157454	-1.182615	-1.08293
F	-0.44114	-1.446203	1.062422
F	0.957229	1.429307	-0.292633
F	1.064148	0.522616	1.686709
F	2.376001	-0.458996	-1.390806
F	2.165856	-1.763758	0.346752
O	4.983695	-1.535586	-0.295981
O	5.681013	0.587612	-0.424638
O	3.793118	2.572834	0.04743
H	4.67566	2.268287	-0.250818
F	-5.173725	-0.292041	0.14744

m=7

Charge = -1 Multiplicity = 2

C	4.737311	-0.110083	-0.232843
C	3.418433	0.323911	0.44455
C	2.171654	-0.355002	-0.174406
C	0.863531	0.411583	0.147241
C	-0.39678	-0.47352	-0.032108
C	-1.691151	0.362486	-0.193761
C	-2.985901	-0.44046	0.09001
C	-4.217425	0.181537	-0.500799
H	-4.129967	0.242365	-1.583479
H	-4.282823	1.30141	-0.129063
C	-5.556684	-0.456862	-0.101734
F	4.75851	-1.428949	-0.37492
F	4.85976	0.458765	-1.420777
F	3.489627	-0.001407	1.737572
F	3.309794	1.653317	0.328981
F	2.084467	-1.599885	0.30997
F	2.32216	-0.415163	-1.503148
F	0.91639	0.840112	1.414646
F	0.781038	1.468569	-0.669868
F	-0.506888	-1.268219	1.039165
F	-0.228236	-1.231804	-1.12476
F	-1.62658	1.404321	0.653363

F	-1.721725	0.835395	-1.449197
F	-3.077169	-0.559327	1.433401
F	-2.785185	-1.686164	-0.415481
O	-5.523974	-1.585484	0.429537
O	-6.568216	0.222513	-0.381369
O	-4.294485	2.654567	0.095322
H	-3.544634	2.896743	-0.475628
F	5.756579	0.259903	0.52587

m=8

Charge = -1 Multiplicity = 2

C	-5.371542	-0.248644	-0.099098
C	-4.052837	0.552462	-0.168996
C	-2.815589	-0.289941	0.228533
C	-1.492624	0.329518	-0.288271
C	-0.254837	-0.207811	0.475476
C	1.061419	-0.002132	-0.317269
C	2.315288	-0.071672	0.591138
C	3.623304	-0.36149	-0.179249
C	4.861573	-0.05109	0.6114
H	4.832952	-0.531702	1.587026
H	4.843777	1.128537	0.806268
C	6.143225	-0.371053	-0.177579
F	-5.455246	-1.095233	-1.111946
F	-5.429565	-0.923678	1.041477
F	-4.153051	1.591571	0.66362
F	-3.905886	1.002524	-1.420932
F	-2.769269	-0.370748	1.563903
F	-2.943314	-1.52215	-0.277321
F	-1.54952	1.658052	-0.135455
F	-1.365185	0.042229	-1.58887
F	-0.169211	0.432372	1.647594
F	-0.420726	-1.517044	0.701612
F	1.022728	1.201449	-0.906388
F	1.134402	-0.945905	-1.263096
F	2.424019	1.102182	1.229932
F	2.134944	-1.039682	1.505181
F	3.58314	0.35937	-1.327812
F	3.590293	-1.667965	-0.536458
O	6.653751	0.562575	-0.837562
O	6.550731	-1.54637	-0.089556

O	5.095824	2.415981	0.552533
H	5.786859	2.180507	-0.101073
F	-6.391921	0.592244	-0.15749

m=9

Charge = -1 Multiplicity = 2

C	6.01546	-0.260233	0.095351
C	4.696977	0.542471	0.162225
C	3.465166	-0.297358	-0.274278
C	2.133049	0.293152	0.250762
C	0.85958	-0.364604	-0.337326
C	-0.434549	0.413484	0.037594
C	-1.700985	-0.473296	-0.088071
C	-3.002793	0.359336	-0.20388
C	-4.282908	-0.446099	0.134714
C	-5.537919	0.169606	-0.411781
H	-5.493981	0.216603	-1.497866
H	-5.58669	1.29495	-0.052684
C	-6.858968	-0.467527	0.045763
F	6.094446	-0.912335	-1.056841
F	6.08048	-1.127326	1.092421
F	7.035263	0.578349	0.189133
F	4.80583	1.591072	-0.658937
F	4.549173	0.985879	1.414628
F	3.58434	-1.544294	0.201429
F	3.46599	-0.339883	-1.609292
F	2.109499	0.119714	1.577064
F	2.106971	1.604082	-0.030665
F	0.783852	-1.615083	0.137469
F	0.935876	-0.40533	-1.670076
F	-0.34714	0.865195	1.29297
F	-0.544544	1.459904	-0.791044
F	-1.767448	-1.261379	0.992131
F	-1.57779	-1.239012	-1.181545
F	-2.912267	1.406906	0.633002
F	-3.08274	0.823929	-1.460392
F	-4.321605	-0.556626	1.481621
F	-4.099095	-1.694657	-0.369672
O	-6.802119	-1.597014	0.573302
O	-7.882297	0.210818	-0.189219
O	-5.591689	2.654534	0.113762

H	-4.91497	2.876181	-0.549281

(1-3) Formula: F-(CF_2)$_m$-CH_2-$PO4^{2-}$

m=1

Charge = -2 Multiplicity = 2

C	-2.037017	-0.253758	0.009442
C	-0.65857	0.085162	0.504536
H	-0.58716	-0.096291	1.578449
H	-0.562444	1.245709	0.35948
F	-2.200642	0.067277	-1.279821
F	-2.30591	-1.562282	0.119661
O	0.266504	-0.603459	-0.251933
P	1.902228	-0.254758	0.01503
O	2.58171	-1.37264	-0.73577
O	2.061602	-0.260582	1.519056
O	2.077771	1.126436	-0.615244
O	-0.080167	2.531159	-0.029365
H	0.803036	2.127288	-0.281298
F	-2.96819	0.404885	0.70906

m=2

Charge = -2 Multiplicity = 2

C	-1.254087	-0.499033	-0.33878
C	0.024848	-0.011769	0.293847
H	0.003447	-0.13579	1.378595
H	0.049841	1.143927	0.094793
F	-1.282664	-0.198386	-1.656297
F	-1.370379	-1.84303	-0.234904
O	1.082488	-0.648515	-0.322913
P	2.644913	-0.176749	0.134143
O	3.488798	-1.243551	-0.51762
O	2.619999	-0.167516	1.646342
O	2.794513	1.211682	-0.486905
O	0.460064	2.435631	-0.349933
H	1.402155	2.103834	-0.442831
C	-2.51819	0.102928	0.28595
F	-2.633455	-0.27201	1.555576
F	-3.597258	-0.307751	-0.371704
F	-2.473073	1.430582	0.236156

m=3

Charge = -2 Multiplicity = 2

C	-3.145764	-0.211752	-0.004169
C	-1.764266	0.406819	0.290834
C	-0.567539	-0.399563	-0.245239
C	0.754766	0.063081	0.317594
H	0.772842	-0.028022	1.404448
H	0.822167	1.211739	0.082388
F	-3.248465	-0.542079	-1.284436
F	-3.343569	-1.291181	0.738065
F	-1.738245	1.62917	-0.259545
F	-1.663785	0.532139	1.623905
F	-0.574098	-0.292892	-1.591299
F	-0.780251	-1.706127	0.048209
O	1.75928	-0.63806	-0.316913
P	3.356884	-0.26534	0.110433
O	4.11804	-1.374432	-0.572049
O	3.365925	-0.273472	1.622715
O	3.575523	1.11854	-0.498818
O	1.317557	2.480774	-0.345669
H	2.236523	2.090679	-0.440809
F	-4.089206	0.676236	0.283903

m=4

Charge = -2 Multiplicity = 2

C	3.655481	0.1551	-0.141404
C	2.3305	-0.625929	0.000012
C	1.077713	0.266105	-0.168725
C	-0.205661	-0.359072	0.418463
C	-1.482144	0.231466	-0.135627
H	-1.535047	0.05943	-1.212973
H	-1.439194	1.374864	0.002293
F	3.877475	0.896305	0.932614
F	3.611775	0.939135	-1.211178
F	2.322841	-1.19732	1.211462
F	2.316507	-1.581324	-0.935251
F	1.311169	1.441652	0.438593
F	0.905067	0.494337	-1.479455
F	-0.152522	-0.213906	1.759422
F	-0.165917	-1.690794	0.161277

O	-2.540671	-0.305191	0.567156
P	-4.058231	-0.217621	-0.196369
O	-4.964049	-0.730262	0.901265
O	-3.925531	-1.126893	-1.40282
O	-4.210484	1.25127	-0.54177
O	-1.328781	2.856676	0.215129
H	-0.78427	2.799243	1.019755
F	4.655024	-0.703643	-0.278767

m=5

Charge = -2 Multiplicity = 2

C	-1.759476	-0.419218	-0.102242
C	-0.419514	0.290278	0.214067
C	0.818299	-0.459991	-0.31665
C	2.108196	0.029298	0.297276
H	2.103049	-0.095943	1.380804
H	2.136606	1.185441	0.094138
F	-1.718318	-0.930778	-1.33875
F	-1.936018	-1.419612	0.77201
F	-0.442363	1.518453	-0.329069
F	-0.323296	0.414813	1.546548
F	0.849042	-0.311746	-1.657459
F	0.637266	-1.780354	-0.065318
O	3.153699	-0.61205	-0.333794
P	4.723946	-0.22556	0.174385
O	5.542842	-1.240881	-0.583292
O	4.694155	-0.374402	1.679485
O	4.911536	1.21453	-0.297775
O	2.589365	2.471188	-0.332064
H	3.529836	2.125238	-0.357407
C	-2.972728	0.53819	-0.014981
C	-4.320092	-0.203269	0.126529
F	-2.833519	1.347011	1.042971
F	-3.024011	1.27524	-1.128291
F	-4.450757	-0.706705	1.343002
F	-4.392721	-1.184777	-0.763126
F	-5.308591	0.65066	-0.091161

m=6

Charge = -2 Multiplicity = 2

C	4.886552	0.189267	-0.00123

C	3.56245	-0.579927	-0.208635
C	2.314489	0.327819	-0.086589
C	1.017688	-0.482356	0.165506
C	-0.259595	0.322564	-0.183125
C	-1.538271	-0.234914	0.478528
C	-2.817328	0.230492	-0.180553
H	-2.837445	-0.082352	-1.226865
H	-2.809016	1.384608	-0.19044
F	5.06697	0.465624	1.279785
F	4.866249	1.320528	-0.693621
F	3.499766	-1.554416	0.707236
F	3.584894	-1.122566	-1.42863
F	2.497562	1.181929	0.928233
F	2.187003	1.023696	-1.223529
F	0.985997	-0.834734	1.456337
F	1.054062	-1.589479	-0.588656
F	-0.078859	1.593212	0.214013
F	-0.40853	0.308692	-1.516097
F	-1.51604	0.12206	1.78027
F	-1.461362	-1.588738	0.434931
O	-3.876758	-0.242301	0.564019
P	-5.377321	-0.31258	-0.23453
O	-6.283478	-0.742183	0.898273
O	-5.17313	-1.344748	-1.327409
O	-5.588005	1.098883	-0.746535
O	-2.822849	2.85716	0.086888
H	-2.285227	2.817068	0.897183
F	5.894438	-0.557228	-0.424408

m=7

Charge = -2 Multiplicity = 2

C	5.484709	-0.280258	-0.345141
C	4.211353	0.375445	0.232654
C	2.921716	-0.417871	-0.092408
C	1.646607	0.448971	0.061676
C	0.365527	-0.409414	0.219889
C	-0.924611	0.388705	-0.09263
C	-2.201964	-0.257523	0.489192
C	-3.475826	0.180991	-0.198673
H	-3.461984	-0.139439	-1.242936
H	-3.499165	1.332978	-0.223183

F	5.483821	-1.579907	-0.079542
F	5.54652	-0.10242	-1.654451
F	4.349018	0.450101	1.55867
F	4.115771	1.611885	-0.271074
F	2.846139	-1.461991	0.741927
F	2.99044	-0.869404	-1.350251
F	1.784944	1.224392	1.144517
F	1.52599	1.225269	-1.02168
F	0.313462	-0.857764	1.480271
F	0.446961	-1.453551	-0.615729
F	-0.784283	1.623085	0.420244
F	-1.044668	0.49082	-1.424192
F	-2.24127	0.034055	1.805988
F	-2.067268	-1.603941	0.384299
O	-4.54044	-0.316011	0.522871
P	-6.030593	-0.386584	-0.293739
O	-6.946756	-0.835002	0.823664
O	-5.808832	-1.404998	-1.395988
O	-6.244689	1.02944	-0.791418
O	-3.471333	2.834707	-0.208198
H	-2.976199	2.914567	0.625484
F	6.548599	0.275068	0.213439

m=8

Charge = -2 Multiplicity = 2

C	-6.148641	0.239588	-0.233859
C	-4.858738	-0.291691	0.428795
C	-3.573238	0.358153	-0.139806
C	-2.307586	-0.481626	0.167282
C	-1.005588	0.350895	0.045302
C	0.249051	-0.543442	-0.124121
C	1.560931	0.202388	0.22654
C	2.822502	-0.458037	-0.366216
C	4.096529	0.013047	0.29381
H	4.095938	-0.220662	1.359016
H	4.089586	1.184692	0.212457
F	-6.122289	1.565064	-0.273474
F	-6.269762	-0.232079	-1.463577
F	-4.809984	-1.616195	0.240477
F	-4.930459	-0.034511	1.737236
F	-3.696445	0.485527	-1.465915

F	-3.43529	1.573661	0.403281
F	-2.254623	-1.504361	-0.693944
F	-2.399227	-0.960131	1.413818
F	-1.109162	1.159279	-1.016753
F	-0.86896	1.093004	1.150528
F	0.300293	-0.966849	-1.392259
F	0.126864	-1.604649	0.685543
F	1.479039	1.461559	-0.233656
F	1.669681	0.243085	1.563086
F	2.846182	-0.190422	-1.688299
F	2.686085	-1.80128	-0.234028
O	5.161052	-0.529691	-0.395386
P	6.719964	-0.116314	0.125996
O	7.567495	-1.073594	-0.674137
O	6.698789	-0.328313	1.624089
O	6.858729	1.34821	-0.28403
O	4.51066	2.528497	-0.022457
H	5.45651	2.214564	-0.136452
F	-7.192681	-0.151857	0.479497

m=9

Charge = -2 Multiplicity = 2

C	6.775678	0.003099	-0.346346
C	5.475853	0.280335	0.441368
C	4.214547	-0.276569	-0.262783
C	2.911314	0.378409	0.261165
C	1.656416	-0.471055	-0.066183
C	0.348508	0.357724	0.017712
C	-0.906991	-0.539432	0.16442
C	-2.21338	0.201614	-0.216709
C	-3.485097	-0.459974	0.3524
C	-4.747608	0.007811	-0.331923
H	-4.726789	-0.227135	-1.396705
H	-4.744406	1.179643	-0.251675
F	6.85736	0.796418	-1.401524
F	6.799518	-1.261429	-0.746892
F	7.815814	0.226873	0.440677
F	5.353765	1.604615	0.592728
F	5.587751	-0.292441	1.642051
F	4.156198	-1.596378	-0.047262
F	4.313515	-0.053316	-1.578321

F	3.002718	0.520845	1.588425
F	2.779895	1.584801	-0.302073
F	1.586615	-1.485302	0.803637
F	1.779129	-0.961674	-1.30535
F	0.424511	1.17541	1.075074
F	0.234671	1.090113	-1.09656
F	-0.984207	-0.9583	1.432727
F	-0.764713	-1.603319	-0.638406
F	-2.144112	1.462769	0.240193
F	-2.294918	0.236783	-1.555371
F	-3.534813	-0.190682	1.673431
F	-3.343403	-1.803092	0.224316
O	-5.823118	-0.536726	0.338406
P	-7.373996	-0.121886	-0.204567
O	-8.232983	-1.079999	0.582251
O	-7.332444	-0.331167	-1.702612
O	-7.518273	1.341984	0.206064
O	-5.16888	2.523448	-0.025376
H	-6.116365	2.209437	0.074809

(1-4) Formula: F-(CF_2)$_m$-CH_2-$SO3^-$

m=1

Charge = -1 Multiplicity = 2

C	1.451624	-0.258993	-0.065623
C	0.209135	0.233179	-0.746694
H	0.234022	0.011654	-1.810628
H	0.218614	1.434491	-0.643925
F	1.424343	-0.07887	1.258437
F	1.663506	-1.562952	-0.281274
S	-1.346479	-0.275944	-0.00575
O	-1.221852	-1.714824	0.214846
O	-1.450865	0.49925	1.232806
O	-2.34534	0.091705	-1.005164
O	0.139182	2.627558	-0.102393
H	-0.400114	2.358689	0.665527
F	2.52966	0.390226	-0.528921

m=2

Charge = -1 Multiplicity = 2

C	-2.105772	-0.067785	0.255878
C	-0.700919	-0.329003	-0.31191
C	0.395893	0.311041	0.497144
H	0.228062	0.219158	1.568311
H	0.407354	1.492447	0.272632
F	-2.34675	1.236216	0.330168
F	-2.219199	-0.592919	1.470548
F	-0.717994	0.112075	-1.588178
F	-0.562932	-1.674367	-0.358802
S	2.063694	-0.240238	0.107254
O	2.163353	-1.574523	0.697172
O	2.156344	-0.234361	-1.350955
O	2.915658	0.750684	0.759991
O	0.373281	2.779148	-0.023956
H	-0.235783	2.754159	-0.783135
F	-3.022351	-0.622678	-0.529131

m=3

Charge = -1 Multiplicity = 2

C	-2.580387	-0.185507	-0.278159

C	-1.308855	-0.131228	0.594075
C	-0.135915	0.657225	-0.033997
C	1.181287	0.44122	0.672245
H	1.059416	0.250664	1.736275
H	1.770243	1.484831	0.604164
F	-2.896625	1.021213	-0.728139
F	-2.404411	-0.998969	-1.308814
F	-1.632493	0.455055	1.756138
F	-0.944507	-1.394846	0.840938
F	-0.485781	1.963968	0.036592
F	-0.075013	0.339289	-1.34506
S	2.335915	-0.734155	-0.061138
O	1.580522	-1.956335	-0.31736
O	2.813395	-0.074698	-1.279359
O	3.366284	-0.873063	0.963927
O	2.516746	2.485525	0.154261
H	2.883196	2.000472	-0.609705
F	-3.587818	-0.644731	0.453981

m=4

Charge = -1 Multiplicity = 2

C	-3.332133	-0.119025	0.23887
C	-1.989199	-0.01608	-0.517192
C	-0.773782	0.141786	0.427753
C	0.57892	-0.214529	-0.229498
C	1.749018	0.290024	0.574916
H	1.602649	0.163261	1.6465
H	1.833827	1.47677	0.403052
F	-3.404238	0.822614	1.170852
F	-3.456464	-1.30655	0.810007
F	-2.053817	1.050238	-1.3218
F	-1.855331	-1.118409	-1.264613
F	-0.74266	1.416663	0.842529
F	-0.949382	-0.649159	1.498573
F	0.565452	0.309359	-1.477051
F	0.615339	-1.558166	-0.363839
S	3.357394	-0.365609	0.106535
O	3.344632	-1.759692	0.548015
O	3.438636	-0.208462	-1.343831
O	4.297147	0.471595	0.847507
O	1.921385	2.742008	0.038464

H	1.91648	2.627613	-0.92842
F	-4.328077	0.04735	-0.618663

m=5

Charge = -1 Multiplicity = 2

C	-2.648798	-0.218524	0.516852
C	-1.358496	-0.05922	-0.323222
C	-0.094548	0.094007	0.558892
C	1.22456	-0.220315	-0.185044
C	2.431257	0.287703	0.560834
H	2.352442	0.131928	1.635354
H	2.489621	1.479097	0.414893
F	-2.612358	0.623194	1.557754
F	-2.720409	-1.474139	0.96753
F	-1.480545	1.02855	-1.096563
F	-1.234817	-1.135734	-1.108739
F	-0.056161	1.355909	1.009291
F	-0.199708	-0.733388	1.610967
F	1.128937	0.332987	-1.416658
F	1.279017	-1.559235	-0.354182
S	4.017668	-0.330461	-0.021299
O	4.065028	-1.72541	0.415316
O	3.994554	-0.168643	-1.473309
O	4.988872	0.525119	0.655548
O	2.512234	2.760166	0.096149
H	2.232274	2.693963	-0.833821
C	-3.934787	0.074059	-0.287657
F	-4.067903	1.373992	-0.49495
F	-3.892903	-0.55274	-1.456015
F	-4.982889	-0.358699	0.396098

m=6

Charge = -1 Multiplicity = 2

C	2.008079	-0.089736	-0.396529
C	0.696642	0.054417	0.415865
C	-0.553732	0.152224	-0.493925
C	-1.878048	-0.181159	0.231489
C	-3.083459	0.292995	-0.540499
H	-2.963435	0.197342	-1.617244
H	-3.216479	1.458368	-0.293104
F	1.953835	0.712617	-1.467241

F	2.125455	-1.357774	-0.809319
F	0.777186	1.16626	1.159901
F	0.583406	-1.003967	1.226285
F	-0.617323	1.401986	-0.976118
F	-0.407706	-0.696201	-1.524158
F	-1.82069	0.392346	1.455465
F	-1.9042	-1.518603	0.41891
S	-4.647583	-0.445006	-0.040954
O	-4.621891	-1.794364	-0.602829
O	-4.648051	-0.414438	1.420201
O	-5.650123	0.422948	-0.653415
O	-3.230136	2.761772	-0.076364
H	-2.798528	3.051083	-0.899157
C	3.259358	0.29076	0.432916
F	3.363926	1.621796	0.468947
F	3.131339	-0.17427	1.681539
C	4.568857	-0.276586	-0.158575
F	4.608278	-0.05367	-1.465816
F	4.65561	-1.577611	0.064355
F	5.599238	0.32581	0.413869

m=7

Charge = -1 Multiplicity = 2

C	5.101148	-0.121552	-0.169228
C	3.728919	-0.447083	0.460289
C	2.561994	0.342026	-0.181764
C	1.183107	-0.298542	0.122952
C	0.013339	0.698818	-0.082912
C	-1.350184	-0.020094	-0.259618
C	-2.564955	0.9025	0.005423
C	-3.869968	0.430576	-0.57768
H	-3.847179	0.458592	-1.664815
H	-4.674377	1.259376	-0.263883
F	5.201207	-0.65497	-1.375432
F	5.257415	1.192685	-0.257432
F	3.508353	-1.759972	0.319578
F	3.791286	-0.146627	1.760126
F	2.73764	0.378499	-1.507891
F	2.582966	1.593095	0.29449
F	1.015543	-1.349376	-0.688486
F	1.17519	-0.720756	1.393459

F	0.266487	1.428664	-1.17801
F	-0.039825	1.510204	0.979974
F	-1.410683	-0.47987	-1.516365
F	-1.395356	-1.053593	0.593548
F	-2.263047	2.10767	-0.544145
F	-2.647416	1.084928	1.337771
S	-4.557841	-1.137679	-0.027285
O	-3.738585	-2.158839	-0.678468
O	-4.452272	-1.13791	1.429437
O	-5.932133	-1.090374	-0.520521
O	-5.456337	2.239368	0.19613
H	-5.259975	2.158838	1.146387
F	6.055931	-0.620778	0.600089

m=8

Charge = -1 Multiplicity = 2

C	5.831362	-0.352637	-0.00356
C	4.53699	0.458839	0.224608
C	3.270179	-0.273966	-0.281107
C	1.97262	0.293176	0.348427
C	0.710024	-0.08192	-0.470458
C	-0.590585	0.047961	0.362534
C	-1.856294	0.134089	-0.528045
C	-3.165274	-0.207909	0.222162
C	-4.389404	0.239277	-0.535519
H	-4.29737	0.095943	-1.60971
H	-4.514274	1.414753	-0.333119
F	5.90745	-1.355558	0.855393
F	5.849648	-0.831964	-1.240414
F	4.653978	1.61834	-0.426812
F	4.420258	0.697384	1.536454
F	3.205527	-0.140824	-1.611534
F	3.367213	-1.573471	0.022668
F	2.068684	1.626871	0.406353
F	1.851359	-0.191657	1.589556
F	0.633311	0.730832	-1.53101
F	0.828555	-1.346205	-0.893922
F	-0.508904	1.159527	1.1068
F	-0.682787	-1.01264	1.172588
F	-1.938643	1.381674	-1.012789
F	-1.719798	-0.716078	-1.558065

F	-3.094582	0.381447	1.43757
F	-3.171078	-1.54329	0.42545
S	-5.947437	-0.458543	0.036015
O	-5.923672	-1.853118	-0.403011
O	-5.939491	-0.297936	1.4881
O	-6.954889	0.349974	-0.645692
O	-4.527733	2.722834	-0.152286
H	-4.105441	2.990139	-0.987234
F	6.876992	0.440097	0.168679

m=9

Charge = -1 Multiplicity = 2

C	6.485765	0.312045	0.028551
C	5.189006	-0.525066	-0.036027
C	3.91453	0.317135	0.216643
C	2.634827	-0.385472	-0.303338
C	1.348034	0.181403	0.349933
C	0.077326	-0.149315	-0.474759
C	-1.218901	-0.022851	0.36605
C	-2.482867	0.116357	-0.519221
C	-3.799592	-0.22306	0.21596
C	-5.004221	0.264795	-0.543299
H	-4.924988	0.089985	-1.614092
H	-5.04809	1.458312	-0.400588
F	6.469399	1.087375	1.105034
F	6.606098	1.067163	-1.051011
F	7.524771	-0.504517	0.099703
F	5.265197	-1.481347	0.892223
F	5.117319	-1.08984	-1.24757
F	4.039923	1.497249	-0.40116
F	3.796565	0.524173	1.533676
F	2.562865	-0.216241	-1.628827
F	2.717614	-1.692812	-0.03083
F	1.463916	1.510855	0.450157
F	1.222843	-0.341749	1.574882
F	0.00995	0.694974	-1.510949
F	0.174496	-1.402883	-0.934263
F	-1.115378	1.061052	1.14706
F	-1.331362	-1.108255	1.1398
F	-2.547064	1.383058	-0.955842
F	-2.360508	-0.698772	-1.578461

F	-3.723115	0.336023	1.444208
F	-3.841293	-1.563066	0.383981
S	-6.591252	-0.345052	0.049683
O	-6.725534	-1.679987	-0.528418
O	-6.508693	-0.337097	1.507496
O	-7.543742	0.626845	-0.491241
O	-5.413137	2.709214	-0.255138
H	-6.37161	2.542937	-0.331123

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(2-1) Formula: F-$(CF_2)_{7-m}$-(CH_2)-$(CF_2)_m$-OH

m=1

Charge = 0 Multiplicity = 2

C	-4.391944	-0.230294	0.158559
C	-3.070533	0.301825	-0.439209
C	-1.827812	-0.086464	0.399358
C	-0.51239	0.025786	-0.412322
C	0.736643	0.121417	0.499295
C	2.056525	-0.236383	-0.221257
C	3.268605	0.238775	0.542818
H	3.149252	0.167468	1.620988
H	3.39387	1.417621	0.278929
C	4.569889	-0.392118	0.10799
O	5.606829	0.305674	0.612971
H	6.440631	-0.132263	0.382311
F	4.622293	-1.691361	0.513875
F	4.635427	-0.455801	-1.251665
F	2.078929	-1.577412	-0.384777
F	2.008925	0.312538	-1.45645
F	0.580029	-0.713165	1.538544
F	0.816325	1.375456	0.965738
F	-0.409338	-1.048497	-1.202969
F	-0.574742	1.125045	-1.175842
F	-1.965236	-1.346372	0.829863
F	-1.763016	0.730026	1.458569
F	-2.947811	-0.188665	-1.678606
F	-3.15016	1.633658	-0.500043
F	-4.49881	-1.534632	-0.034415
F	-4.43439	0.023683	1.45994
F	-5.409194	0.375252	-0.433601
O	3.47736	2.682287	0.038923
H	3.065745	3.010443	0.857783

m=2

Charge = 0 Multiplicity = 2

C	-4.422117	0.118626	-0.241312
C	-3.117961	-0.05223	0.568931
C	-1.856627	-0.135765	-0.324808
C	-0.55453	0.145839	0.46657

C	0.715562	-0.386275	-0.231703
C	1.982085	0.199235	0.349394
C	3.215944	-0.595647	-0.015884
C	4.538683	0.183821	0.122625
O	5.567744	-0.671677	0.066017
H	6.407124	-0.186588	0.098876
F	4.594988	1.108614	-0.860144
F	4.514496	0.878502	1.28551
F	0.605838	-0.099476	-1.548049
F	0.715074	-1.732022	-0.112422
F	-0.442961	1.470687	0.627047
F	-0.648479	-0.428295	1.675389
F	-1.965708	0.764357	-1.311038
F	-1.801692	-1.36017	-0.86254
F	-3.007667	0.990187	1.401999
F	-3.219398	-1.177002	1.282763
F	-4.513779	1.347226	-0.722834
F	-4.447761	-0.747958	-1.245529
F	-5.457453	-0.10831	0.552008
F	3.152428	-1.046469	-1.288538
F	3.297169	-1.682755	0.786425
H	2.056551	1.331548	-0.121133
H	1.923683	0.338817	1.426463
O	2.116357	2.57201	-0.41243
H	2.757734	2.853899	0.263801

m=3

Charge = 0 Multiplicity = 2

C	0.658125	0.216345	0.416414
C	1.937566	-0.289853	-0.211916
C	3.179802	0.08364	0.626924
C	4.523357	-0.029488	-0.12441
F	4.6016	0.974426	-1.022501
F	4.525276	-1.175477	-0.842515
F	3.210969	-0.725508	1.696543
F	3.053891	1.349959	1.0572
H	0.609279	1.416802	0.175297
H	0.675062	0.172342	1.503623
F	2.093248	0.20522	-1.45858
F	1.909926	-1.637647	-0.325445
O	0.562438	2.629349	-0.225261

H	0.365679	2.492448	-1.169361
C	-0.577231	-0.459645	-0.127033
C	-1.883772	0.311539	0.184962
F	-1.808165	0.826632	1.42
F	-2.018252	1.317152	-0.69247
F	-0.505722	-0.615753	-1.463986
F	-0.702245	-1.69488	0.416023
C	-3.148208	-0.577776	0.10904
C	-4.452602	0.238571	-0.030983
O	5.519395	0.01439	0.768456
H	6.376063	0.003805	0.313039
F	-3.239769	-1.305746	1.226237
F	-3.06177	-1.398362	-0.945744
F	-4.460675	1.235797	0.844426
F	-4.567073	0.731179	-1.253608
F	-5.487124	-0.553138	0.208179

m=4

Charge = 0 Multiplicity = 2

C	-4.487241	-0.359497	0.177016
C	-3.185094	0.468648	0.142381
C	-1.912481	-0.374038	-0.095573
C	-0.643879	0.340354	0.308728
C	0.588156	-0.244733	-0.34606
C	1.894163	0.148617	0.382094
C	3.163389	-0.063763	-0.480014
C	4.467216	-0.139954	0.343504
O	5.505418	-0.024402	-0.491207
H	6.339827	-0.144399	-0.010069
F	4.43853	0.839936	1.276813
F	4.485663	-1.30404	1.02321
F	-1.892179	-0.713001	-1.400618
F	-2.042637	-1.520991	0.612909
F	-3.297467	1.364579	-0.844801
F	-3.08539	1.117559	1.311079
F	-4.527717	-1.198261	-0.850142
F	-4.576852	-1.048901	1.303824
F	-5.525155	0.462072	0.099688
F	3.25899	0.959028	-1.339074
F	3.043994	-1.203261	-1.178298
F	1.830287	1.444901	0.721006

F	1.98428	-0.578155	1.505823
H	-0.718798	1.500795	-0.089803
H	-0.564704	0.402575	1.391355
F	0.687292	0.164138	-1.629832
F	0.521686	-1.594946	-0.359368
O	-0.724546	2.748505	-0.339458
H	-0.338593	3.078488	0.491396

m=5

Charge = 0 Multiplicity = 2

C	-1.977806	0.12229	0.374891
C	-0.71711	-0.358511	-0.308772
C	0.552773	-0.021801	0.509284
C	1.854646	-0.08452	-0.328204
F	1.938925	1.031131	-1.064778
F	1.798131	-1.141371	-1.150122
F	0.643773	-0.891631	1.52736
F	0.435296	1.214542	1.012427
H	-2.001565	1.341611	0.210846
H	-1.941682	0.002304	1.45637
F	-0.586266	0.199378	-1.532404
F	-0.744429	-1.696984	-0.48731
O	-1.923925	2.555029	-0.166229
H	-2.289744	2.475157	-1.065517
C	-3.234931	-0.484993	-0.192796
C	-4.528514	0.189397	0.294774
F	-5.57818	-0.481649	-0.162996
F	-4.571107	0.194011	1.621681
F	-4.602797	1.438041	-0.142599
F	-3.246624	-0.433496	-1.540624
F	-3.336003	-1.785167	0.165396
C	3.121643	-0.214467	0.553886
C	4.421964	0.198777	-0.170754
O	5.464921	-0.238947	0.541724
H	6.295388	0.084588	0.156994
F	4.428453	1.538746	-0.316461
F	4.392787	-0.315855	-1.422108
F	2.982438	0.562477	1.639294
F	3.229341	-1.488768	0.946963

m=6

Charge = 0 Multiplicity = 2

C	-4.561563	-0.386852	0.074714
C	-3.252233	0.142148	0.594805
C	-2.043808	-0.273104	-0.207805
C	-0.72461	0.093069	0.509319
C	0.521521	0.02978	-0.410144
C	1.841631	-0.079864	0.395535
C	3.07961	0.333803	-0.439695
C	4.410656	-0.203477	0.131236
O	5.420498	0.451406	-0.449586
H	6.271005	0.081447	-0.162586
F	4.389502	-0.042753	1.475034
F	4.469046	-1.532493	-0.086584
F	-4.726557	-0.141055	-1.228722
F	-4.669548	-1.709404	0.243656
F	-5.581119	0.178453	0.724322
F	3.129931	1.670127	-0.475893
F	2.939938	-0.127676	-1.691841
F	1.763189	0.723189	1.465721
F	1.981675	-1.343945	0.812606
F	0.559903	1.142896	-1.155064
F	0.425839	-1.031521	-1.219871
F	-0.554373	-0.7545	1.535584
F	-0.824135	1.338791	0.993018
H	-3.330157	1.36364	0.53771
H	-3.148603	-0.075538	1.656405
F	-2.031802	0.317931	-1.422355
F	-2.04318	-1.608356	-0.413264
O	-3.509747	2.601863	0.290004
H	-3.760246	2.554148	-0.649793

m=7

Charge = 0 Multiplicity = 2

C	4.865947	-0.099157	-0.371423
C	3.599466	-0.529018	0.294294
C	2.319231	-0.102117	-0.456673
C	1.030143	-0.201726	0.396654
C	-0.255607	-0.243901	-0.469461
C	-1.52274	0.139316	0.337944

F	-1.55697	1.471329	0.464465
F	-1.442575	-0.410137	1.557439
F	-0.125258	0.613672	-1.489806
F	-0.40475	-1.482278	-0.956914
F	0.967411	0.864893	1.206638
F	1.072383	-1.311432	1.143969
F	2.181728	-0.883085	-1.541477
F	2.447175	1.170101	-0.863752
H	4.990984	1.07854	-0.206331
H	4.864717	-0.284011	-1.441454
F	3.515399	-0.034022	1.554541
F	3.563483	-1.881194	0.400169
O	5.048533	2.399525	-0.100645
H	4.563918	2.615532	-0.915699
H	5.721659	-0.538893	0.134667
C	-2.826683	-0.350471	-0.340381
C	-4.088768	0.391992	0.151745
F	-2.723046	-0.172958	-1.666336
F	-2.964117	-1.656849	-0.088473
F	-4.069319	1.646408	-0.341952
F	-4.009743	0.515472	1.496869
O	-5.168253	-0.291427	-0.239194
H	-5.975635	0.185268	0.012934

(2-2) Formula: $F\text{-}(CF_2)_{7-m}\text{-}(CH_2)\text{-}(CF_2)_m\text{-}COO^-$

m=1

Charge = -1 Multiplicity = 2

C	-4.788251	-0.172664	0.204471
C	-3.463062	0.409783	-0.333043
C	-2.214699	-0.13898	0.40073
C	-0.916473	0.061317	-0.421419
C	0.357721	-0.015636	0.456658
C	1.644315	-0.302517	-0.348705
C	2.889094	0.023814	0.439376
H	2.80195	-0.242856	1.491026
H	2.950389	1.241613	0.428753
C	4.170784	-0.525175	-0.14637
C	5.436888	0.149836	0.459614
O	6.01761	-0.478956	1.353396
O	5.705778	1.274972	-0.014714
F	-5.796913	0.539618	-0.272907
F	-4.934832	-1.430448	-0.177676
F	-4.803047	-0.11245	1.529573
F	-3.504184	1.736194	-0.181119
F	-3.380782	0.116815	-1.636623
F	-2.381625	-1.446708	0.632417
F	-2.099429	0.498603	1.572324
F	-0.963155	1.265275	-1.007958
F	-0.86757	-0.882491	-1.368675
F	0.198679	-0.984383	1.371583
F	0.494372	1.15731	1.092351
F	1.575177	0.426613	-1.486878
F	1.619372	-1.604573	-0.710058
F	4.216073	-1.869153	0.062401
F	4.170959	-0.357717	-1.499055
O	3.213706	2.485115	0.225075
H	4.16514	2.340981	0.024994

m=2

Charge = -1 Multiplicity = 2

C	-4.797638	0.109187	-0.208129
C	-3.497444	-0.260271	0.541083
C	-2.229342	-0.085045	-0.329267

C	-0.936848	0.00658	0.518753
C	0.34905	-0.277947	-0.292785
C	1.590793	0.217598	0.40982
C	2.870853	-0.356127	-0.151976
F	0.205589	0.305788	-1.50417
F	0.412809	-1.611698	-0.500421
F	-0.866297	1.239471	1.038356
F	-1.014859	-0.878962	1.524217
F	-2.354392	1.038063	-1.049381
F	-2.144537	-1.127897	-1.164095
F	-3.408433	0.520563	1.625187
F	-3.587445	-1.536322	0.924896
F	-4.909862	1.42236	-0.322858
F	-4.795921	-0.435994	-1.417681
F	-5.836526	-0.351316	0.470988
F	2.818128	-0.425969	-1.500959
F	3.023782	-1.628792	0.302169
H	1.586049	1.432817	0.278915
H	1.545592	0.076876	1.487603
O	1.512587	2.675065	-0.041745
H	1.902159	2.633744	-0.933202
C	4.141076	0.422901	0.241779
C	5.430666	-0.432796	0.065413
F	3.990305	0.830178	1.521915
F	4.202052	1.535553	-0.526429
O	5.915258	-0.900744	1.106708
O	5.80086	-0.557214	-1.114598

m=3

Charge = -1 Multiplicity = 2

C	4.84438	0.267322	-0.142629
C	3.544122	-0.544657	0.043432
C	2.271435	0.271124	-0.299438
C	0.982413	-0.308466	0.323967
C	-0.275114	0.297834	-0.256023
C	-1.528129	-0.468451	0.105365
C	-2.830142	0.339399	-0.113117
C	-4.10602	-0.515906	-0.245747
C	-5.38835	0.345557	-0.030916
O	-5.952187	0.211159	1.064573
O	-5.667587	1.081796	-0.992156

F	5.879186	-0.558976	-0.116852
F	4.823742	0.897336	-1.310076
F	4.982676	1.154177	0.829532
F	3.504734	-0.967621	1.312021
F	3.604487	-1.606921	-0.766615
F	2.151511	0.288267	-1.634221
F	2.427269	1.531906	0.131846
F	1.045491	-0.095302	1.65399
F	1.012374	-1.64846	0.127891
F	-4.112918	-1.0747	-1.475981
F	-4.026317	-1.518399	0.655531
F	-2.69136	1.086338	-1.222934
F	-2.987516	1.168308	0.936104
H	-0.216048	0.448347	-1.330001
H	-0.319533	1.420923	0.237307
F	-1.601024	-1.583975	-0.66232
F	-1.502184	-0.873981	1.391764
O	-0.395107	2.614646	0.68902
H	-1.024293	2.985415	0.044719

m=4

Charge = -1 Multiplicity = 2

C	-4.900903	-0.208207	-0.055713
C	-3.54623	0.13714	0.595915
C	-2.302576	-0.267863	-0.218165
C	-1.031479	0.291911	0.377744
C	0.211749	-0.399648	-0.131872
C	1.502832	0.427933	0.084466
C	2.79498	-0.424297	0.066223
C	4.079239	0.397304	-0.172291
C	5.34612	-0.389186	0.28438
O	5.883029	0.009217	1.32706
O	5.639931	-1.339356	-0.460299
F	-5.867857	0.040664	0.818074
F	-5.104702	0.532884	-1.134075
F	-4.949027	-1.488991	-0.392345
F	-3.494496	-0.483185	1.782536
F	-3.526291	1.462321	0.796132
F	-2.475415	0.156811	-1.487418
F	-2.260122	-1.619165	-0.249689
F	4.149214	0.687885	-1.48985

F	3.950677	1.564504	0.494053
F	2.684505	-1.354418	-0.896088
F	2.904092	-1.047243	1.25345
F	1.580775	1.351744	-0.886244
F	1.419734	1.053776	1.2688
F	0.113994	-0.673366	-1.448825
F	0.367168	-1.580812	0.513513
H	-1.000276	1.481483	0.084484
H	-1.045256	0.302471	1.465859
O	-0.964618	2.6877	-0.333793
H	-0.773823	2.534343	-1.276434

m=5

Charge = -1 Multiplicity = 2

C	-4.901089	0.090868	0.377987
C	-3.611541	-0.331911	-0.342668
C	-2.36149	0.241184	0.280325
C	-1.107076	-0.492305	-0.135974
C	0.177059	0.341608	0.085644
C	1.469012	-0.512427	0.127525
C	2.747684	0.330302	-0.109177
C	4.04275	-0.347816	0.379284
C	5.302427	0.330732	-0.243362
O	5.861125	-0.299051	-1.151827
O	5.567177	1.440066	0.24878
F	-5.953198	-0.412715	-0.253979
F	-4.899423	-0.359917	1.626139
F	-5.00975	1.413308	0.399723
F	-3.738068	0.047612	-1.629915
F	-3.587507	-1.684379	-0.321813
F	4.075779	-0.26609	1.726849
F	3.963341	-1.655603	0.052051
F	2.604605	1.509122	0.517939
F	2.858255	0.558224	-1.429258
F	1.55023	-1.103819	1.327785
F	1.394636	-1.459749	-0.818196
F	0.068604	1.002623	1.24755
F	0.279503	1.231783	-0.912228
F	-0.983883	-1.634712	0.580786
F	-1.155104	-0.838694	-1.437875
H	-2.424912	0.316204	1.362748

H	-2.274494	1.397416	-0.130323
O	-2.224303	2.644556	-0.376972
H	-2.69118	2.977466	0.410218

m=6

Charge = -1 Multiplicity = 2

C	4.946046	-0.367301	-0.129239
C	3.631677	0.215654	-0.573528
C	2.41797	-0.325644	0.137365
C	1.109246	0.351775	-0.334537
C	-0.16803	-0.440794	0.046061
C	-1.442058	0.443576	0.011082
C	-2.744993	-0.3862	-0.095219
C	-4.010699	0.392257	0.319706
C	-5.2985	-0.290775	-0.235388
O	-5.855156	0.289311	-1.177339
O	-5.584404	-1.35478	0.338479
F	5.949102	0.208542	-0.796752
F	5.180181	-0.190647	1.173253
F	5.013515	-1.682784	-0.3678
F	-4.041892	0.444654	1.66897
F	-3.880232	1.657423	-0.132904
F	-2.619529	-1.4746	0.680963
F	-2.884826	-0.783529	-1.371297
F	-1.47895	1.17591	1.132568
F	-1.365501	1.266847	-1.044488
F	-0.029237	-0.945214	1.278413
F	-0.3171	-1.450749	-0.822309
F	1.042984	1.574581	0.212096
F	1.135469	0.476109	-1.66905
H	3.711972	1.417569	-0.340812
H	3.540039	0.150707	-1.654915
F	2.512874	-0.153339	1.47044
F	2.288214	-1.655316	-0.088456
O	3.90781	2.595218	0.106825
H	3.812401	2.427453	1.061357

m=7

Charge = -1 Multiplicity = 2

C	5.115127	-0.697535	0.34248
C	3.925749	0.090113	-0.095346

C	2.582803	-0.606209	0.221596
C	1.343336	0.314374	0.087359
C	0.02392	-0.486533	-0.061294
C	-1.227239	0.361089	0.284466
C	-2.53392	-0.240139	-0.291343
C	-3.811236	0.280708	0.397723
C	-5.077019	0.01002	-0.473646
O	-5.554467	0.995464	-1.052181
O	-5.429264	-1.181025	-0.485539
F	-3.917768	-0.334744	1.594929
F	-3.636455	1.599092	0.631527
F	-2.477577	-1.576029	-0.16836
F	-2.59494	0.067315	-1.597905
F	-1.328753	0.438981	1.618067
F	-1.060212	1.59523	-0.211675
F	0.063265	-1.545444	0.758355
F	-0.074927	-0.915646	-1.326356
F	1.258157	1.081695	1.183686
F	1.482371	1.104505	-0.98379
F	2.617559	-1.065071	1.482074
F	2.440061	-1.650523	-0.61144
F	3.892648	1.306378	0.50589
F	3.96144	0.306806	-1.431584
H	5.187648	-0.781228	1.422053
H	5.187087	-1.651451	-0.171225
H	6.056123	-0.050754	0.008836
O	7.121808	0.654041	-0.392299
H	6.791571	0.867351	-1.282244

(2-3) Formula: $F\text{-}(CF_2)_{7-m}\text{-}(CH_2)\text{-}(CF_2)_m\text{-}SO_3^-$

m=1

Charge = -1 Multiplicity = 2

C	-5.241835	-0.091406	0.27889
C	-3.92567	0.302068	-0.426811
C	-2.6669	-0.025815	0.413114
C	-1.379306	-0.069981	-0.448084
C	-0.09448	0.077993	0.405922
C	1.179076	-0.42943	-0.305865
C	2.438615	0.076152	0.357816
H	2.368545	0.075444	1.443345
H	2.490312	1.260681	0.055815
C	3.685316	-0.641147	-0.093459
F	3.762296	-1.849127	0.515228
F	3.672206	-0.874463	-1.424785
F	1.143956	-1.780166	-0.305723
F	1.107934	-0.026656	-1.594432
F	-0.250622	-0.607268	1.548729
F	0.06369	1.375994	0.700387
F	-1.348773	-1.234773	-1.106105
F	-1.424796	0.930947	-1.337138
F	-2.833782	-1.215436	1.004178
F	-2.533	0.914026	1.357348
F	-3.867994	-0.351239	-1.593719
F	-3.960137	1.61666	-0.659007
F	-5.40075	-1.404656	0.271961
F	-5.227667	0.341942	1.532681
F	-6.25798	0.466193	-0.360036
O	2.628616	2.466537	-0.345136
H	3.581883	2.398369	-0.560422
S	5.244371	0.260041	0.303219
O	5.222763	1.409479	-0.602688
O	6.291979	-0.704447	0.009638
O	5.09154	0.602983	1.71

m=2

Charge = -1 Multiplicity = 2

C	-5.271918	0.064315	-0.177765
C	-3.95528	-0.283903	0.552319

C	-2.700551	-0.072695	-0.329441
C	-1.401827	0.035063	0.507651
C	-0.119297	-0.222473	-0.317289
C	1.121477	0.283159	0.381476
C	2.401487	-0.286162	-0.18926
C	3.656792	0.526139	0.196986
F	3.733891	1.592097	-0.618697
F	3.516888	0.977515	1.457616
F	-0.279958	0.373034	-1.520509
F	-0.03889	-1.552471	-0.540338
F	-1.347529	1.265642	1.034435
F	-1.454703	-0.858567	1.507348
F	-2.85439	1.056083	-1.034796
F	-2.603943	-1.103478	-1.17764
F	-3.870358	0.487128	1.643767
F	-4.013586	-1.565698	0.923267
F	-5.411151	1.37548	-0.285213
F	-5.2761	-0.476053	-1.389397
F	-6.29231	-0.418995	0.513545
F	2.343385	-0.344535	-1.537127
F	2.558584	-1.554597	0.258432
H	1.107411	1.500065	0.251261
H	1.084175	0.140723	1.459466
O	1.040956	2.741676	-0.059503
H	1.37947	2.70033	-0.971704
S	5.255229	-0.398618	0.084917
O	6.240619	0.669299	0.170238
O	5.236913	-1.293314	1.231342
O	5.177952	-1.054807	-1.211826

m=3

Charge = -1 Multiplicity = 2

C	0.167729	0.227795	-0.292254
C	-1.07766	-0.241165	0.427473
C	-2.368593	0.130032	-0.338325
C	-3.650391	0.025062	0.515676
F	-3.720663	1.113677	1.298777
F	-3.568005	-1.057263	1.309734
F	-2.461692	-0.682335	-1.402467
F	-2.251236	1.393333	-0.77779
H	0.252054	1.437316	-0.103104

H	0.084663	0.147609	-1.374264
F	-1.155253	0.293136	1.666414
F	-1.055552	-1.585154	0.576596
O	0.351854	2.667378	0.221987
H	0.568304	2.574322	1.166924
C	1.423947	-0.451304	0.197825
C	2.717962	0.299548	-0.201295
F	2.577482	0.794196	-1.438951
F	2.909761	1.31846	0.649289
F	1.42421	-0.578193	1.539885
F	1.506421	-1.699258	-0.323583
C	3.977366	-0.599761	-0.180169
C	5.293882	0.20714	-0.12124
F	4.003204	-1.34333	-1.290262
F	3.941781	-1.405509	0.88914
F	5.262019	1.196434	-1.005066
F	5.480519	0.710472	1.08821
F	6.306865	-0.595802	-0.410127
S	-5.214171	-0.087957	-0.467922
O	-5.068767	0.974772	-1.45099
O	-6.23411	0.145203	0.542601
O	-5.196787	-1.436327	-1.010742

m=4

Charge = -1 Multiplicity = 2

C	-5.346713	-0.165863	-0.081742
C	-3.999198	-0.036944	0.658925
C	-2.761259	-0.271623	-0.232441
C	-1.491179	0.234112	0.412279
C	-0.242696	-0.333513	-0.219836
C	1.038028	0.464643	0.132254
C	2.340644	-0.358229	-0.037262
C	3.599901	0.529949	-0.142405
F	-6.327459	-0.21823	0.809372
F	-5.54685	0.879122	-0.87004
F	-5.371516	-1.272506	-0.812347
F	-3.986272	-0.933175	1.653465
F	-3.945413	1.194231	1.185714
F	-2.981096	0.337001	-1.418666
F	-2.686032	-1.598184	-0.479043
F	3.651943	1.040072	-1.382593

F	3.489475	1.549246	0.728712
F	2.239198	-1.092514	-1.155503
F	2.45915	-1.179957	1.013997
F	1.104339	1.540744	-0.667337
F	0.956925	0.879331	1.404785
F	-0.348228	-0.370727	-1.563404
F	-0.061306	-1.60728	0.205131
H	-1.511349	1.453848	0.27731
H	-1.477912	0.091205	1.490828
O	-1.594304	2.682527	-0.058495
H	-1.307416	2.623277	-0.98754
S	5.187308	-0.364482	0.189239
O	5.190405	-0.56334	1.628852
O	5.054276	-1.578489	-0.601478
O	6.181229	0.579754	-0.296036

m=5

Charge = -1 Multiplicity = 2

C	-2.803434	0.102127	0.410329
C	-1.554073	-0.286244	-0.348094
C	-0.264701	0.065634	0.429011
C	1.007023	0.058045	-0.457286
F	1.043032	1.201146	-1.156672
F	0.941653	-0.971147	-1.312451
F	-0.11465	-0.824124	1.422264
F	-0.399383	1.286329	0.965184
H	-2.905292	1.322481	0.317102
H	-2.711763	-0.061085	1.482964
F	-1.498522	0.334364	-1.546787
F	-1.539477	-1.615979	-0.587823
O	-2.956793	2.573619	0.082124
H	-3.252803	2.555304	-0.845435
C	-4.045098	-0.568999	-0.12367
C	-5.363706	0.076754	0.340391
F	-6.380155	-0.721939	0.039325
F	-5.346738	0.267459	1.654184
F	-5.554859	1.241147	-0.262908
F	-4.068752	-0.577649	-1.472737
F	-4.08763	-1.855462	0.290364
C	2.312214	-0.067042	0.370232
C	3.561402	0.385277	-0.417947

F	3.591743	1.726686	-0.41809
F	3.449824	-0.034206	-1.691503
F	2.194387	0.694853	1.468057
F	2.448424	-1.345744	0.743043
S	5.159468	-0.242143	0.276007
O	5.025871	0.016	1.701283
O	6.14101	0.583285	-0.409152
O	5.178727	-1.64632	-0.097952

m=6

Charge = -1 Multiplicity = 2

C	5.397804	-0.321171	-0.028855
C	4.096409	0.135784	-0.631921
C	2.875133	-0.421263	0.05512
C	1.584186	0.373374	-0.262037
C	0.29164	-0.449681	-0.032603
C	-0.963556	0.448129	0.118034
C	-2.2822	-0.329779	-0.131458
C	-3.513946	0.377847	0.473649
F	6.420354	0.025091	-0.812212
F	5.621568	0.210134	1.176059
F	5.432798	-1.652688	0.116304
F	-3.52073	0.147645	1.79526
F	-3.393124	1.703137	0.275956
F	-2.166492	-1.547034	0.419623
F	-2.441135	-0.464879	-1.453908
F	-0.977989	0.952524	1.358932
F	-0.884945	1.455819	-0.761351
F	0.428313	-1.178144	1.082958
F	0.114274	-1.271458	-1.075336
F	1.543169	1.458586	0.525524
F	1.613836	0.768683	-1.541552
H	4.111307	1.357274	-0.566571
H	4.070517	-0.064685	-1.700267
F	3.022996	-0.442186	1.394334
F	2.677978	-1.701377	-0.345141
S	-5.130607	-0.186751	-0.23324
O	-5.17941	0.438834	-1.543524
O	-6.088957	0.335758	0.727246
O	-4.998093	-1.63559	-0.243831
O	4.202422	2.613283	-0.360703

H	4.089529	2.623047	0.606559

m=7

Charge = -1 Multiplicity = 2

C	-5.683095	-0.216867	0.405583
C	-4.409527	-0.602363	-0.274233
C	-3.137015	-0.130809	0.462706
C	-1.854029	-0.185485	-0.403822
C	-0.55827	-0.181848	0.448652
C	0.685218	0.249049	-0.371876
F	0.673227	1.583497	-0.488637
F	0.608871	-0.296324	-1.593188
F	-0.7101	0.668402	1.472234
F	-0.358825	-1.414595	0.932108
F	-1.837988	0.883128	-1.213795
F	-1.865244	-1.295767	-1.151351
F	-2.962164	-0.904677	1.547098
F	-3.305345	1.136866	0.869418
H	-5.850114	0.956144	0.245411
H	-5.6645	-0.405189	1.47488
F	-4.356742	-0.104329	-1.535031
F	-4.327784	-1.952374	-0.381333
O	-5.972916	2.272914	0.145833
H	-5.475935	2.509121	0.947676
H	-6.528453	-0.68414	-0.093152
C	2.01787	-0.189911	0.288591
C	3.22998	0.610004	-0.237003
F	1.914622	-0.00439	1.612868
F	2.194934	-1.49418	0.045456
F	3.229571	1.810248	0.362327
F	3.083483	0.79874	-1.561095
S	4.866182	-0.201957	0.068971
O	4.77842	-0.609382	1.462991
O	4.905503	-1.291341	-0.891384
O	5.800077	0.879879	-0.197898

(2-4) Formula: $F\text{-}(CF_2)_{7-m}\text{-}(CH_2)\text{-}(CF_2)_m\text{-}PO_4^{2-}$

m=1

Charge = -2 Multiplicity = 2

C	5.56942	-0.273984	-0.277663
C	4.283005	0.293994	0.361548
C	3.001989	-0.085759	-0.421614
C	1.722125	0.056952	0.439413
C	0.436477	0.146043	-0.420711
C	-0.855029	-0.178076	0.36246
C	-2.088996	0.269534	-0.377804
H	-2.022728	0.090413	-1.448542
H	-2.134287	1.474079	-0.25903
C	-3.401516	-0.264266	0.162555
O	-4.418008	0.457708	-0.299173
F	-3.510908	-1.587624	-0.169821
F	-3.360188	-0.26509	1.533634
F	-0.879723	-1.51155	0.582471
F	-0.750836	0.423991	1.569636
F	0.54366	-0.709534	-1.449164
F	0.344723	1.392851	-0.906452
F	1.641256	-0.998795	1.257385
F	1.82864	1.171793	1.175369
F	3.105959	-1.352819	-0.840527
F	2.90583	0.718534	-1.487746
F	4.200416	-0.173056	1.613262
F	4.389827	1.624689	0.395378
F	5.666902	-1.573575	-0.050899
F	5.557194	-0.058304	-1.58659
F	6.620292	0.333046	0.250979
O	-2.445244	2.720018	-0.074025
H	-3.413541	2.61353	-0.098784
P	-6.07106	-0.106847	-0.282565
O	-6.777924	1.222043	-0.411406
O	-6.149077	-0.998894	-1.499186
O	-6.221716	-0.809996	1.045477

m=2

Charge = -2 Multiplicity = 2

C	-5.573359	0.227566	-0.215383

C	-4.285917	-0.160639	0.545157
C	-3.014717	-0.081039	-0.33484
C	-1.715941	-0.012957	0.505977
C	-0.448928	-0.403829	-0.291709
C	0.816341	0.07315	0.383972
C	2.074379	-0.568026	-0.152168
C	3.384692	0.076039	0.344725
O	4.424503	-0.62159	-0.067474
F	3.396559	1.367264	-0.082455
F	3.295617	0.145765	1.70603
F	-0.567031	0.116542	-1.534056
F	-0.457839	-1.747993	-0.426993
F	-1.581799	1.237035	0.96788
F	-1.834734	-0.844568	1.55298
F	-3.089935	1.013575	-1.103827
F	-2.982186	-1.162345	-1.123618
F	-4.160483	0.665348	1.59146
F	-4.428736	-1.412569	0.988693
F	-5.621141	1.535226	-0.410711
F	-5.613299	-0.3915	-1.387974
F	-6.626023	-0.135981	0.500797
F	2.09034	-0.539814	-1.504792
F	2.114632	-1.87181	0.218874
H	0.846196	1.283119	0.180499
H	0.766204	-0.011125	1.467656
O	0.736669	2.487892	-0.243494
H	1.269628	2.421875	-1.055789
P	6.049014	0.052653	-0.058473
O	6.087566	0.878112	1.203352
O	6.098778	0.837738	-1.347185
O	6.847234	-1.226255	-0.045228

m=3

Charge = -2 Multiplicity = 2

C	-0.492703	0.190639	0.335532
C	0.763485	-0.386507	-0.28384
C	2.022984	0.003386	0.518328
C	3.380369	-0.231439	-0.183069
F	3.455965	0.628762	-1.231397
F	3.340163	-1.4773	-0.737174
F	2.001751	-0.70107	1.66323

F	1.941827	1.310405	0.829762
H	-0.506378	1.377647	0.023886
H	-0.460295	0.202829	1.42278
F	0.905381	0.033958	-1.558964
F	0.695425	-1.737442	-0.32036
O	-0.513586	2.544061	-0.504085
H	-0.893455	2.335957	-1.377233
C	-1.759761	-0.460933	-0.159904
C	-3.038505	0.32727	0.215633
F	-2.916073	0.798847	1.464064
F	-3.176969	1.365596	-0.622533
F	-1.745169	-0.60251	-1.500636
F	-1.89032	-1.699374	0.374759
C	-4.325143	-0.531128	0.149292
C	-5.613224	0.317928	0.065958
O	4.356231	-0.08365	0.688906
F	-4.405644	-1.285848	1.249454
F	-4.286769	-1.3261	-0.927599
F	-5.575913	1.29047	0.967992
F	-5.749206	0.846965	-1.13924
F	-6.659017	-0.456978	0.311354
P	6.023886	0.179043	0.178025
O	6.05567	1.656518	-0.127439
O	6.730323	-0.24029	1.441801
O	6.178606	-0.735741	-1.010658

m=4

Charge = -2 Multiplicity = 2

C	-5.611336	-0.507758	0.208546
C	-4.352358	0.383471	0.251206
C	-3.059669	-0.343366	-0.189625
C	-1.802287	0.318453	0.316941
C	-0.558021	-0.120432	-0.423401
C	0.729056	0.22069	0.360706
C	2.016656	0.160757	-0.496812
C	3.32081	0.008818	0.322801
O	4.358674	0.272279	-0.439117
F	3.210356	0.847013	1.395392
F	3.331331	-1.246765	0.841408
F	-3.073185	-0.411265	-1.536551
F	-3.132652	-1.614743	0.273934

F	-4.566907	1.423469	-0.562843
F	-4.212707	0.835144	1.505318
F	-5.666007	-1.165609	-0.942756
F	-5.610184	-1.377055	1.206833
F	-6.688895	0.257564	0.316472
F	2.084451	1.293036	-1.21301
F	1.935142	-0.874772	-1.349984
F	0.608221	1.46322	0.855626
F	0.823211	-0.635577	1.389892
H	-1.89034	1.533996	0.171272
H	-1.714006	0.20079	1.39515
F	-0.480249	0.46545	-1.63821
F	-0.57689	-1.456699	-0.627979
O	-1.987996	2.774549	-0.112925
H	-2.229928	2.712078	-1.054268
P	5.997609	-0.202503	0.02359
O	6.774798	0.803907	-0.785047
O	6.012226	-0.015294	1.519911
O	6.080761	-1.629794	-0.456577

m=5

Charge = -2 Multiplicity = 2

C	-3.114642	0.178271	0.368163
C	-1.882877	-0.375412	-0.314642
C	-0.586641	-0.02771	0.455212
C	0.697213	-0.185567	-0.397804
F	0.801341	0.882206	-1.200373
F	0.581621	-1.285081	-1.15717
F	-0.506469	-0.833363	1.526072
F	-0.659603	1.241306	0.880526
H	-3.124121	1.382188	0.111473
H	-3.049006	0.138975	1.454004
F	-1.768173	0.108857	-1.570799
F	-1.949157	-1.720722	-0.415394
O	-3.044645	2.562729	-0.360578
H	-3.426089	2.418987	-1.245469
C	-4.39869	-0.443304	-0.117503
C	-5.669019	0.270442	0.377006
F	-6.738569	-0.419776	-0.000062
F	-5.662953	0.354443	1.702097
F	-5.754938	1.491062	-0.131169

F	-4.458587	-0.465388	-1.46535
F	-4.502112	-1.720072	0.316101
C	1.975005	-0.315113	0.466212
C	3.29365	-0.010959	-0.286107
O	4.313629	-0.441891	0.420213
F	3.323376	1.323371	-0.533912
F	3.195792	-0.608097	-1.511695
F	1.882358	0.531211	1.507091
F	2.024802	-1.56828	0.939743
P	5.957075	0.164607	0.171397
O	5.964494	1.436161	0.982276
O	6.052056	0.338508	-1.323552
O	6.724531	-0.990288	0.760951

m=6

Charge = -2 Multiplicity = 2

C	5.689464	-0.473241	-0.010275
C	4.434186	0.214233	0.456756
C	3.176893	-0.286324	-0.211493
C	1.899204	0.174688	0.526492
C	0.617676	0.061155	-0.337778
C	-0.676807	0.039337	0.514554
C	-1.936137	0.401551	-0.311921
C	-3.269483	-0.077164	0.310804
F	6.769084	0.199268	0.392509
F	5.789584	-1.713674	0.48009
F	5.745493	-0.569463	-1.342315
F	-3.301395	-1.430238	0.208073
F	-3.196703	0.187455	1.64965
F	-1.827099	-0.144822	-1.535455
F	-1.96953	1.734756	-0.443826
F	-0.812038	-1.183782	1.04216
F	-0.548643	0.927053	1.512353
F	0.671625	-1.065472	-1.060089
F	0.573607	1.110514	-1.17035
F	1.754227	-0.573345	1.630599
F	2.047926	1.455128	0.893107
H	4.378544	0.213547	1.542452
H	4.56178	1.376366	0.104893
F	3.162888	-1.636574	-0.257564
F	3.101209	0.156796	-1.48629

O	-4.274505	0.524377	-0.28276
P	-5.921301	-0.119891	-0.226025
O	-6.032941	-0.692927	1.163924
O	-5.920884	-1.122369	-1.353739
O	-6.681066	1.154974	-0.489497
O	4.681264	2.612455	-0.185044
H	4.452149	2.988591	0.68325

m=7

Charge = -2 Multiplicity = 2

C	-5.991006	0.036052	-0.506789
C	-4.765457	-0.434123	0.207764
C	-3.442244	-0.050886	-0.489581
C	-2.184649	-0.225505	0.398465
C	-0.878147	-0.298032	-0.434629
C	0.383666	0.014684	0.409656
C	1.684872	-0.498898	-0.255401
C	2.978407	0.170229	0.267171
F	2.966378	1.462709	-0.148678
F	2.869141	0.221828	1.627498
F	1.606658	-0.285809	-1.580394
F	1.762893	-1.81939	-0.039464
F	0.453857	1.340271	0.582969
F	0.251441	-0.571374	1.608787
F	-0.951129	0.587313	-1.437582
F	-0.768068	-1.530711	-0.947471
F	-2.104533	0.816879	1.237912
F	-2.292863	-1.350647	1.115627
F	-3.501356	1.23476	-0.868189
F	-3.304387	-0.81338	-1.587855
F	-4.712151	0.054761	1.47255
F	-4.783213	-1.786999	0.310369
H	-6.069338	1.231343	-0.43075
H	-5.967674	-0.18892	-1.569686
H	-6.879327	-0.344632	-0.010303
O	4.023901	-0.509064	-0.1471
P	5.648173	0.190943	-0.130778
O	5.683516	0.983516	-1.413829
O	5.665462	1.006171	1.137163
O	6.457926	-1.079263	-0.123821
O	-6.143233	2.536571	-0.224833

H	-5.45351	2.611562	0.457123

(3-1) Formula: F-$(CF_2)_{8-m}$-$(CH_2)_m$-OH

m=2(α)

Charge = 0 Multiplicity = 2

C	-4.068739	-0.073672	0.135804
C	-2.706147	0.566735	-0.20788
C	-1.51919	-0.416596	-0.059334
C	-0.158485	0.314755	0.063521
C	1.042383	-0.606351	-0.268966
C	2.391304	-0.098952	0.28574
C	3.580045	-0.777096	-0.336689
C	4.879769	-0.377495	0.340957
H	4.881378	-0.597718	1.406046
H	5.024498	0.752007	0.248508
F	-4.187987	-0.24266	1.442381
F	-4.183294	-1.248312	-0.470033
F	-2.52646	1.614769	0.605412
F	-2.75862	0.994938	-1.471963
F	-1.709117	-1.165205	1.034423
F	-1.496894	-1.215237	-1.133814
F	-0.040521	0.77665	1.313958
F	-0.155207	1.352181	-0.785949
O	5.989277	-1.018821	-0.228157
H	5.974698	-0.881156	-1.182598
F	-5.037872	0.725383	-0.282476
O	5.321094	2.185123	-0.221131
H	4.384777	2.430263	-0.315542
H	3.442477	-1.856303	-0.247484
H	3.612047	-0.515669	-1.394351
F	0.801575	-1.8266	0.239171
F	1.122949	-0.709239	-1.603781
F	2.367995	-0.286913	1.626669
F	2.420289	1.246933	0.081648

m=2(β)

Charge = 0 Multiplicity = 2

C	-3.980177	0.337668	0.283908
C	-2.737603	-0.37226	-0.297498
C	-1.414237	0.356893	0.041253
C	-0.177392	-0.564155	-0.111577

C	1.141976	0.234969	-0.251995
C	2.411143	-0.591581	0.062499
C	3.680753	0.025372	-0.447357
H	4.522466	-0.720196	-0.070501
H	3.723845	-0.018706	-1.533425
C	4.018865	1.385435	0.114616
H	3.375341	2.147545	-0.332425
H	3.877828	1.39781	1.19697
F	-4.059614	0.139895	1.589526
F	-3.911038	1.640312	0.042595
F	-5.067797	-0.151466	-0.29045
F	-2.703778	-1.617492	0.192657
F	-2.873631	-0.425722	-1.62479
F	-1.472759	0.802078	1.302475
F	-1.287829	1.404063	-0.783431
F	-0.107113	-1.360532	0.961282
F	-0.343536	-1.319931	-1.205857
F	1.099349	1.284765	0.586796
F	1.218248	0.69331	-1.509594
F	2.456996	-0.755601	1.404468
F	2.233054	-1.818141	-0.486081
O	5.378236	1.630497	-0.217367
H	5.619676	2.497069	0.125569
O	5.678496	-1.191021	0.487385
H	6.142057	-0.333233	0.474214

m=3(α)

Charge = 0 Multiplicity = 2

C	3.823067	-0.097049	-0.103817
C	2.457165	0.586155	0.122346
C	1.263512	-0.397952	0.049261
C	-0.082724	0.322639	-0.207422
C	-1.327265	-0.506105	0.17546
C	-2.601803	0.027569	-0.41533
C	-3.819395	-0.717243	0.120943
C	-5.077127	-0.231835	-0.565707
H	-5.045406	-0.388265	-1.643641
H	-5.155484	0.894783	-0.423576
F	3.980026	-0.418484	-1.377673
F	3.91116	-1.193571	0.637154
F	2.31721	1.540159	-0.807238

F	2.477043	1.153084	1.332584
F	1.484502	-1.271557	-0.943713
F	1.207614	-1.069655	1.206191
F	-0.136652	0.629852	-1.512777
F	-0.096347	1.466744	0.499378
O	-6.248838	-0.841955	-0.083668
H	-6.242392	-0.796925	0.879353
F	4.787936	0.739895	0.246763
O	-5.146629	2.364689	0.153502
H	-4.493261	2.158566	0.844018
H	-3.717747	-1.789887	-0.053801
H	-3.917331	-0.557304	1.196115
H	-2.531293	-0.075875	-1.497854
H	-2.662487	1.091676	-0.180216
F	-1.093659	-1.784369	-0.225998
F	-1.381437	-0.5294	1.530499

m=3(β)

Charge = 0 Multiplicity = 2

C	3.676784	0.404193	0.128174
C	2.404504	-0.449519	0.324342
C	1.109003	0.277953	-0.10898
C	-0.06897	-0.699889	-0.346423
C	-1.459529	-0.03313	-0.289522
C	-2.548751	-0.883872	-0.889347
C	-3.93825	-0.317445	-0.633068
H	-3.873462	0.847468	-0.566193
H	-4.596963	-0.492288	-1.481555
C	-4.581763	-0.785399	0.64803
H	-4.752876	-1.864234	0.588171
H	-3.937645	-0.58608	1.505577
F	3.992939	0.483946	-1.154176
F	3.483115	1.62627	0.606324
F	4.681565	-0.160186	0.780789
F	2.549543	-1.573825	-0.388699
F	2.313052	-0.759968	1.620942
F	1.350855	0.947162	-1.245373
F	0.78562	1.157606	0.846854
F	0.106175	-1.263241	-1.551834
F	-0.020698	-1.667444	0.585781
F	-1.357912	1.156032	-0.940195

F	-1.706445	0.25782	1.01059
O	-5.818447	-0.091411	0.785353
H	-6.214768	-0.339456	1.626274
H	-2.348565	-0.949626	-1.95609
H	-2.466549	-1.888813	-0.467621
O	-4.181934	2.155182	-0.062664
H	-4.964563	1.84796	0.431671

m=3(γ)

Charge = 0 Multiplicity = 2

C	-3.679219	0.158214	-0.270141
C	-2.396731	-0.136823	0.537067
C	-1.11686	-0.146346	-0.334727
C	0.172967	0.019906	0.506085
C	1.454553	-0.450517	-0.214203
C	2.718278	0.05841	0.420665
C	3.969427	-0.512038	-0.209653
H	3.989437	-1.592663	-0.049949
H	3.964979	-0.332336	-1.285765
C	5.213261	0.09865	0.403705
H	5.228438	1.177294	0.230934
H	5.22251	-0.077009	1.482082
F	-3.724337	1.43191	-0.625705
F	-3.715163	-0.600686	-1.357349
F	-4.735817	-0.112068	0.481196
F	-2.2873	0.797726	1.489997
F	-2.538573	-1.335403	1.111223
F	-1.188183	0.858586	-1.218858
F	-1.077308	-1.305067	-1.004832
F	0.292475	1.318061	0.82054
F	0.03879	-0.682772	1.643985
F	1.36206	-0.050584	-1.507696
F	1.430761	-1.806117	-0.221501
O	6.342863	-0.515524	-0.208884
H	7.137985	-0.12592	0.166722
H	2.697249	1.227537	0.254093
H	2.679261	-0.066463	1.503207
O	2.759169	2.538868	-0.175561
H	3.533179	2.44381	-0.757558

m=4(α)

Charge = 0 Multiplicity = 2

C	3.687554	-0.175875	0.061928
C	2.316298	0.53035	-0.009376
C	1.123675	-0.426586	0.229943
C	-0.227664	0.107668	-0.287881
C	-1.417651	-0.630663	0.2566
C	-2.719321	-0.145197	-0.374243
C	-3.916125	-0.866811	0.233074
C	-5.215174	-0.411645	-0.391794
H	-5.233393	-0.56986	-1.47016
H	-5.310265	0.712447	-0.248122
F	3.88911	-0.916436	-1.01694
F	3.749041	-0.948942	1.138673
F	2.218868	1.104551	-1.215377
F	2.301556	1.485828	0.927721
F	1.384343	-1.600042	-0.373534
F	1.04203	-0.644376	1.552476
F	-0.181685	0.039927	-1.642482
F	-0.27559	1.429575	0.032523
O	-6.355669	-1.040148	0.144124
H	-6.296087	-1.008048	1.105628
F	4.645076	0.737746	0.134074
O	-5.313541	2.165946	0.401112
H	-4.556298	1.974694	0.980972
H	-3.817248	-1.945339	0.086542
H	-3.956972	-0.683687	1.310589
H	-2.69561	-0.320955	-1.450446
H	-2.822656	0.930906	-0.221398
H	-1.433988	-0.479938	1.33575
H	-1.268089	-1.694541	0.065039

m=4(β)

Charge = 0 Multiplicity = 2

C	-3.462585	0.560594	-0.094547
C	-2.272908	-0.417483	-0.19921
C	-0.896237	0.273061	-0.04791
C	0.25371	-0.687695	0.320396
C	1.61995	-0.100259	0.103564
C	2.714467	-1.033728	0.62052

C	4.103877	-0.448767	0.447422
H	4.102786	0.61632	0.906175
H	4.84441	-0.996136	1.030785
C	4.567766	-0.294761	-0.978901
H	4.658668	-1.281969	-1.441262
H	3.858239	0.294852	-1.56195
F	-3.63873	0.951737	1.157855
F	-3.250046	1.625186	-0.857711
F	-4.564083	-0.050451	-0.506791
F	-2.432799	-1.351101	0.747466
F	-2.333596	-1.003766	-1.400748
F	-0.986775	1.218585	0.90438
F	-0.619767	0.878678	-1.214086
F	0.065069	-1.04014	1.616943
F	0.07816	-1.817158	-0.417756
O	5.835341	0.361665	-0.954114
H	6.101415	0.542709	-1.860792
H	2.546896	-1.239123	1.676176
H	2.666587	-1.988993	0.09087
O	4.425264	2.055311	0.94553
H	5.125743	1.959455	0.273508
H	1.659842	0.858098	0.624441
H	1.725437	0.089059	-0.963243

m=4(γ)

Charge = 0 Multiplicity = 2

C	-3.555444	-0.303259	-0.011055
C	-2.211334	0.455881	0.020668
C	-0.989125	-0.459644	-0.232561
C	0.351051	0.13159	0.251487
C	1.553987	-0.574119	-0.310764
C	2.855365	-0.060685	0.277405
C	4.064714	-0.802206	-0.25586
H	3.976163	-1.860413	0.006689
H	4.090072	-0.736554	-1.345712
C	5.353911	-0.253016	0.315652
H	5.464938	0.7999	0.046199
H	5.341205	-0.32817	1.405874
F	-3.608037	-1.096075	-1.073801
F	-3.706259	-1.032947	1.083372
F	-4.548722	0.571395	-0.078668

F	-2.252539	1.396951	-0.929521
F	-2.108906	1.050621	1.21617
F	-0.924936	-0.68951	-1.55362
F	-1.19215	-1.633967	0.389862
F	0.342234	1.449906	-0.087052
F	0.338216	0.079803	1.606002
O	6.437516	-1.013359	-0.217042
H	7.258063	-0.65177	0.130848
H	2.989042	1.040952	-0.031565
H	2.835263	-0.052598	1.367383
H	1.544975	-0.451795	-1.393209
H	1.444342	-1.638927	-0.089901
O	3.195077	2.441265	-0.477696
H	2.406337	2.783284	-0.023229

m=4(δ)

Charge = 0 Multiplicity = 2

C	3.447431	0.246145	-0.007526
C	2.155157	-0.594761	-0.099205
C	0.871289	0.265561	-0.167997
C	-0.416777	-0.507716	0.196047
C	-1.68226	0.132616	-0.298694
C	-2.940084	-0.529362	0.223629
C	-4.189601	0.135627	-0.341092
H	-4.207206	1.189604	-0.055854
H	-4.171744	0.089899	-1.432081
C	-5.445879	-0.537484	0.166182
H	-5.454349	-1.58955	-0.12997
H	-5.48245	-0.489637	1.257389
F	3.422625	1.222262	-0.906341
F	3.580939	0.770858	1.200258
F	4.491117	-0.53376	-0.249521
F	2.237729	-1.346697	-1.202539
F	2.113326	-1.395523	0.973854
F	0.767912	0.749156	-1.415765
F	1.009231	1.302903	0.675401
F	-0.29094	-1.75865	-0.326232
F	-0.424443	-0.648163	1.541945
O	-6.572802	0.138245	-0.391689
H	-7.371413	-0.271749	-0.046772
H	-2.921281	-1.585189	-0.063252

H	-2.953507	-0.491594	1.313668
H	-1.65557	0.20232	-1.384504
H	-1.684842	1.244664	0.088077
O	-1.685215	2.600865	0.397217
H	-0.996623	2.863108	-0.238526

(3-2) Formula: $F\text{-}(CF_2)_{8-m}\text{-}(CH_2)_m\text{-}COO^-$

m=2(α)

Charge = -1 Multiplicity = 2

C	-4.519567	-0.193783	0.062424
C	-3.181641	0.528523	-0.207369
C	-1.953737	-0.408259	-0.093613
C	-0.633145	0.374603	0.112718
C	0.619459	-0.466699	-0.241857
C	1.924388	0.060495	0.391461
C	3.166787	-0.517637	-0.228711
H	3.098845	-1.605769	-0.16634
H	3.18845	-0.234122	-1.280352
C	4.416495	-0.034547	0.484504
H	4.477222	1.129124	0.367805
H	4.383777	-0.223552	1.557013
C	5.68426	-0.634083	-0.12474
F	-4.658596	-0.449902	1.352829
F	-4.564589	-1.331981	-0.617119
F	-5.517109	0.583693	-0.329027
F	-3.067994	1.529537	0.67428
F	-3.226841	1.033841	-1.442999
F	-2.132834	-1.237605	0.94222
F	-1.869679	-1.130074	-1.218405
F	-0.57182	0.764726	1.391333
F	-0.658361	1.461971	-0.671892
F	0.422027	-1.730963	0.170092
F	0.742472	-0.469921	-1.577969
F	1.863912	-0.221543	1.715505
F	1.901467	1.415078	0.278261
O	6.476882	0.132883	-0.728076
O	5.828209	-1.868547	0.026374
O	4.950479	2.345158	-0.156799
H	5.708839	1.854974	-0.54302

m=2(β)

Charge = -1 Multiplicity = 2

C	-4.424719	0.268925	-0.15083
C	-3.138706	-0.413149	0.365505
C	-1.850495	0.345276	-0.040217

C	-0.589476	-0.551828	0.040973
C	0.723137	0.267164	0.112439
C	1.982796	-0.548072	-0.265584
C	3.270059	0.03013	0.248186
H	3.325983	1.148304	-0.105609
H	3.245096	0.075608	1.333925
C	4.490572	-0.676093	-0.292009
H	4.455785	-1.733255	-0.013846
H	4.516029	-0.63841	-1.380381
C	5.812077	-0.112618	0.239042
F	-4.568123	0.067361	-1.450403
F	-4.371437	1.573215	0.085885
F	-5.47018	-0.242594	0.479821
F	-3.103722	-1.6576	-0.126946
F	-3.206255	-0.469726	1.698155
F	-1.987431	0.79386	-1.294375
F	-1.703341	1.392551	0.78088
F	-0.564903	-1.339056	-1.041791
F	-0.686376	-1.317642	1.13713
F	0.611963	1.311635	-0.726644
F	0.852886	0.737792	1.361586
F	1.987675	-0.659934	-1.614332
F	1.80812	-1.80443	0.230047
O	5.774385	0.770136	1.128622
O	6.85587	-0.599551	-0.26567
O	3.343157	2.483379	-0.50439
H	2.628443	2.788762	0.081266

m=3(α)

Charge = -1 Multiplicity = 2

C	4.324468	-0.177963	-0.129201
C	2.984509	0.509431	0.215102
C	1.752362	-0.393164	-0.037223
C	0.434599	0.415786	-0.1364
C	-0.8397	-0.421847	0.099543
C	-2.100088	0.26475	-0.346155
C	-3.342452	-0.530173	0.046199
H	-3.279453	-1.541108	-0.362943
H	-3.400619	-0.623204	1.129499
C	-4.594825	0.133566	-0.479789
H	-4.671375	1.186095	-0.024627

H	-4.557682	0.303916	-1.555566
C	-5.923491	-0.516593	-0.100949
F	4.48548	-0.257597	-1.440092
F	4.357581	-1.3984	0.38975
F	5.318864	0.533509	0.38012
F	2.888871	1.61947	-0.528284
F	3.017509	0.848283	1.507431
F	1.938176	-1.060987	-1.185474
F	1.671915	-1.277547	0.964577
F	0.38654	0.963286	-1.361179
F	0.471501	1.407955	0.771
F	-0.660564	-1.602763	-0.552616
F	-0.878118	-0.712535	1.424093
O	-5.911216	-1.432092	0.756946
O	-6.94831	-0.065575	-0.675248
H	-2.118794	1.256713	0.109049
H	-2.043978	0.389989	-1.427133
O	-4.547812	2.611745	0.441053
H	-3.821473	2.848136	-0.16098

m=3(β)

Charge = -1 Multiplicity = 2

C	-4.249348	0.35072	-0.055125
C	-2.993114	-0.543325	0.037093
C	-1.675219	0.265072	0.115736
C	-0.435173	-0.58576	-0.256482
C	0.902243	-0.011004	0.254315
C	2.1071	-0.647719	-0.381583
C	3.407721	-0.130952	0.207168
H	3.506774	0.990293	-0.033886
H	3.411186	-0.17195	1.295727
C	4.618549	-0.812072	-0.387654
H	4.594349	-1.879662	-0.150665
H	4.600404	-0.740189	-1.476779
C	5.962762	-0.268922	0.09776
F	-4.354596	0.886001	-1.260633
F	-4.185783	1.320031	0.848538
F	-5.324049	-0.38702	0.179341
F	-2.971917	-1.335802	-1.042521
F	-3.105841	-1.298729	1.133779
F	-1.758154	1.302324	-0.730302

F	-1.54918	0.737709	1.361649
F	-0.39605	-0.679621	-1.594815
F	-0.59291	-1.820335	0.251882
F	0.865787	1.330192	0.026148
F	0.915668	-0.175618	1.59985
O	5.969281	0.612719	0.991378
O	6.989419	-0.761492	-0.441414
H	2.029266	-1.726612	-0.225737
H	2.067727	-0.459195	-1.454172
O	3.68589	2.293544	-0.729761
H	2.873668	2.220719	-1.259725

m=3(γ)

Charge = -1 Multiplicity = 2

C	4.213925	-0.339202	-0.072805
C	2.906237	0.478023	0.020044
C	1.638421	-0.409295	0.074785
C	0.351702	0.373172	-0.29253
C	-0.951438	-0.294991	0.192087
C	-2.200842	0.284618	-0.409966
C	-3.46271	-0.408287	0.06058
H	-3.417515	-1.455605	-0.244609
H	-3.511182	-0.392777	1.149872
C	-4.703109	0.243649	-0.529376
H	-4.757741	1.295578	-0.244284
H	-4.65542	0.224866	-1.62114
C	-6.020166	-0.418514	-0.128704
F	4.360113	-0.850279	-1.284404
F	4.200138	-1.322891	0.817338
F	5.24075	0.457738	0.181274
F	2.847777	1.284826	-1.047402
F	2.964125	1.221398	1.129053
F	1.788936	-1.425023	-0.787691
F	1.534043	-0.910481	1.311485
F	0.317928	0.487101	-1.629557
F	0.42991	1.603922	0.239258
F	-0.838918	-1.618179	-0.105222
F	-0.980322	-0.196996	1.54204
O	-5.985993	-1.522912	0.469418
O	-7.074301	0.195846	-0.446903
H	-2.219088	1.412384	-0.060744

H	-2.118369	0.332788	-1.49471
O	-2.383095	2.643658	0.561705
H	-3.18603	2.414777	1.061615

m=4(α)

Charge = -1 Multiplicity = 2

C	-4.23896	-0.295409	-0.066814
C	-2.906051	0.483133	-0.03695
C	-1.660633	-0.427074	-0.161874
C	-0.345913	0.228731	0.308436
C	0.887917	-0.503921	-0.136404
C	2.156718	0.132454	0.423613
C	3.397434	-0.610821	-0.059275
H	3.35326	-1.650327	0.277595
H	3.412253	-0.636197	-1.150618
C	4.672978	0.018223	0.45218
H	4.751764	1.087284	0.038344
H	4.664737	0.163712	1.53336
C	5.985674	-0.630684	0.025305
F	-4.42663	-0.950492	1.068246
F	-4.242552	-1.159526	-1.073839
F	-5.23784	0.560016	-0.232781
F	-2.866267	1.17433	1.109333
F	-2.919101	1.343914	-1.061869
F	-1.866776	-1.543986	0.558616
F	-1.548138	-0.775719	-1.453995
F	-0.410787	0.309848	1.661785
F	-0.358485	1.507733	-0.157206
O	5.948729	-1.529416	-0.850745
O	7.030272	-0.198057	0.580244
H	2.210663	1.17693	0.109666
H	2.125977	0.122645	1.514039
H	0.903965	-0.494434	-1.226011
H	0.796157	-1.540805	0.191802
O	4.658932	2.366842	-0.763952
H	3.87195	2.093399	-1.266467

m=4(β)

Charge = -1 Multiplicity = 2

C	-4.136627	0.400513	0.003612
C	-2.888032	-0.503587	0.088296

C	-1.564664	0.290036	0.202794
C	-0.309908	-0.51911	-0.185683
C	0.975627	0.100413	0.28276
C	2.190944	-0.652725	-0.250424
C	3.481117	-0.08451	0.308171
H	3.536185	1.023317	0.02868
H	3.473695	-0.076291	1.399401
C	4.723786	-0.746929	-0.240782
H	4.734353	-1.803798	0.042803
H	4.715471	-0.726621	-1.332421
C	6.047313	-0.143315	0.227679
F	-4.224652	0.967416	-1.189596
F	-4.080609	1.3472	0.931934
F	-5.221258	-0.334066	0.205316
F	-2.872604	-1.277006	-1.005082
F	-3.022621	-1.282102	1.168535
F	-1.640817	1.373152	-0.591009
F	-1.453721	0.708857	1.47354
F	-0.333392	-0.6497	-1.536471
F	-0.471706	-1.769708	0.326198
O	6.025253	0.758795	1.101641
O	7.09271	-0.609782	-0.300655
O	3.538836	2.345287	-0.741687
H	2.773147	2.105637	-1.291657
H	2.121553	-1.708077	0.025768
H	2.211132	-0.603824	-1.340189
H	0.966368	0.093378	1.372487
H	0.988783	1.140785	-0.048081

m=4(γ)

Charge = -1 Multiplicity = 2

C	-4.114921	-0.406097	-0.030074
C	-2.811909	0.420348	0.019904
C	-1.54051	-0.433087	-0.208717
C	-0.240013	0.223512	0.296879
C	1.006449	-0.432476	-0.227911
C	2.268135	0.183711	0.350715
C	3.527336	-0.509702	-0.129958
H	3.473077	-1.562075	0.159675
H	3.559324	-0.487305	-1.221594
C	4.788956	0.115079	0.442972

H	4.846987	1.174818	0.18711
H	4.767264	0.069425	1.535326
C	6.095763	-0.5406	0.000881
F	-4.245319	-1.141516	1.063311
F	-4.111967	-1.202126	-1.092029
F	-5.14991	0.417314	-0.11445
F	-2.762143	1.027009	1.212523
F	-2.884508	1.352885	-0.936991
F	-1.694654	-1.616426	0.410831
F	-1.443287	-0.65966	-1.528689
F	-0.280664	0.183128	1.652418
F	-0.299935	1.535173	-0.055737
O	6.049258	-1.643211	-0.601261
O	7.159188	0.073077	0.291112
H	2.303219	1.281962	0.003408
H	2.231653	0.242398	1.439647
O	2.474977	2.567034	-0.733136
H	3.366694	2.362555	-1.063136
H	0.955989	-1.492852	0.031406
H	1.004184	-0.350274	-1.314384

m=4(δ)

Charge = -1 Multiplicity = 2

C	3.764588	-0.88473	-0.181996
C	2.645431	-0.041574	0.4679
C	1.311784	-0.097669	-0.319634
C	0.337542	1.055818	0.006058
C	-1.061092	0.882282	-0.522463
C	-1.966275	-0.090639	0.204072
C	-3.402766	0.002031	-0.30391
H	-3.773983	1.019884	-0.168325
H	-3.420334	-0.199323	-1.37653
C	-4.31013	-0.976996	0.422935
H	-3.950859	-2.000122	0.284368
H	-4.282859	-0.792558	1.49913
C	-5.775891	-0.959714	-0.004687
F	4.235347	-0.280625	-1.261882
F	3.301457	-2.081333	-0.519731
F	4.754618	-1.037225	0.685495
F	3.0901	1.217388	0.563663
F	2.436602	-0.520631	1.699823

F	1.581705	-0.070351	-1.635967
F	0.735385	-1.274843	-0.032607
F	0.889512	2.177331	-0.521988
F	0.344868	1.207046	1.354192
O	-6.120019	-0.236695	-0.973665
O	-6.561859	-1.695984	0.653936
H	-1.604542	-1.109912	0.057566
H	-1.936443	0.112515	1.276163
H	-1.028285	0.729891	-1.601759
H	-1.502954	1.960865	-0.39617
O	-2.000692	3.195208	0.083519
H	-2.624674	2.814858	0.726614

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(3-3) Formula: $F\text{-}(CF_2)_{8-m}\text{-}(CH_2)_m\text{-}SO_3^-$

m=2(α)

Charge = -1 Multiplicity = 2

C	-5.015275	0.142156	-0.347448
C	-3.741587	-0.195541	0.459158
C	-2.447666	-0.087401	-0.384376
C	-1.177686	0.035932	0.494573
C	0.115104	-0.333731	-0.276144
C	1.403656	0.221154	0.365978
C	2.655652	-0.432234	-0.157094
C	3.880012	0.238636	0.418075
H	3.898842	0.289446	1.504932
H	3.945013	1.352679	0.038321
F	-5.099344	1.445643	-0.557199
F	-4.992833	-0.48822	-1.514501
F	-3.672287	0.647979	1.496456
F	-3.85831	-1.445431	0.915101
F	-2.533796	0.989389	-1.175693
F	-2.351059	-1.182314	-1.149153
F	-1.094686	1.294387	0.941357
F	-1.304906	-0.789335	1.543399
F	0.022677	0.141725	-1.529264
F	0.189372	-1.671835	-0.332248
F	1.424591	1.555831	0.135464
F	1.285933	0.055699	1.708113
S	5.414037	-0.486646	-0.137756
O	5.493227	-1.793051	0.522481
O	5.314854	-0.581276	-1.597028
O	6.447929	0.456697	0.308944
F	-6.079289	-0.25051	0.335159
H	2.651596	-0.367422	-1.24503
H	2.634646	-1.484633	0.129972
O	4.422588	2.589146	-0.33821
H	5.358711	2.363212	-0.182856

m=2(β)

Charge = -1 Multiplicity = 2

C	4.962894	-0.086974	-0.288834
C	3.647808	0.349768	0.393374

C	2.388238	-0.077897	-0.40024
C	1.112997	-0.091144	0.480166
C	-0.188289	-0.033415	-0.358458
C	-1.439123	-0.521594	0.403618
C	-2.72911	-0.10177	-0.247568
C	-3.92824	-0.711273	0.435145
H	-3.935745	-0.518513	1.506667
H	-3.958632	-1.787566	0.263745
F	5.154602	-1.387293	-0.138615
F	4.918417	0.201334	-1.583092
F	3.616527	-0.191688	1.617237
F	3.658304	1.68096	0.502029
F	2.583255	-1.304424	-0.900828
F	2.218524	0.781262	-1.413208
F	1.122755	-1.206978	1.219006
F	1.147335	0.971485	1.296801
S	-5.477911	-0.08274	-0.209335
O	-5.546482	1.335333	0.193417
O	-5.412835	-0.252132	-1.663894
O	-6.514476	-0.894532	0.431736
F	5.974917	0.562087	0.264734
H	-2.701681	-0.283472	-1.32068
H	-2.742279	1.08956	-0.128623
O	-2.962468	2.376752	0.153575
H	-3.935577	2.266024	0.218552
F	-0.031283	-0.794702	-1.453859
F	-0.375298	1.23673	-0.744839
F	-1.356664	-0.046327	1.670792
F	-1.359442	-1.871307	0.48471

m=3(α)

Charge = -1 Multiplicity = 2

C	-4.904109	0.100229	-0.331846
C	-3.626041	-0.013522	0.52844
C	-2.334686	-0.132941	-0.316871
C	-1.062068	0.223139	0.490847
C	0.245212	-0.327761	-0.115349
C	1.479723	0.312438	0.454925
C	2.745735	-0.366618	-0.06235
C	3.966795	0.329162	0.486127
H	3.978746	0.418892	1.5715

H	4.012536	1.426499	0.076326
F	-4.997696	1.304987	-0.870965
F	-4.885161	-0.809754	-1.29715
F	-3.555806	1.073392	1.307911
F	-3.743012	-1.099071	1.299002
F	-2.429993	0.699689	-1.363829
F	-2.249619	-1.388279	-0.773749
F	-0.98914	1.561245	0.563727
F	-1.19387	-0.263647	1.737116
F	0.16753	-0.144285	-1.460344
F	0.24417	-1.667306	0.094907
S	5.523396	-0.377545	-0.022785
O	5.639495	-1.651426	0.697171
O	5.451614	-0.545013	-1.478518
O	6.534784	0.610326	0.387983
F	-5.963576	-0.107263	0.43516
H	2.76883	-0.347391	-1.15135
H	2.764786	-1.411392	0.254908
H	1.467655	1.365764	0.176781
H	1.422313	0.245244	1.54225
O	4.508507	2.67704	-0.331129
H	5.437764	2.433559	-0.159504

m=3(β)

Charge = -1 Multiplicity = 2

C	-4.81518	0.28834	-0.282152
C	-3.549871	-0.262681	0.411388
C	-2.240401	0.140482	-0.310701
C	-0.997269	0.017166	0.603894
C	0.344006	-0.04723	-0.156853
C	1.538287	0.187463	0.727603
C	2.84708	0.019778	-0.024992
C	4.028611	0.407984	0.833223
H	4.141965	-0.259517	1.686864
H	3.92221	1.430618	1.19834
F	-4.945524	1.584437	-0.049451
F	-4.742046	0.08505	-1.591016
F	-3.535988	0.199461	1.66826
F	-3.639064	-1.595529	0.435721
F	-2.35208	1.41092	-0.724513
F	-2.095769	-0.648885	-1.382122

F	-0.988319	1.078074	1.425381
F	-1.122585	-1.096717	1.345812
F	0.281038	0.870454	-1.155289
F	0.402094	-1.265672	-0.754741
S	5.574379	0.370769	-0.061822
O	5.739075	-1.006336	-0.550167
O	5.436806	1.344262	-1.155448
O	6.600228	0.757327	0.917568
F	-5.879314	-0.340123	0.193355
H	2.842879	0.546212	-0.979349
H	2.982732	-1.102852	-0.294642
H	1.463291	1.204876	1.113885
H	1.483818	-0.500707	1.572832
O	3.038747	-2.54632	-0.289681
H	2.080604	-2.683451	-0.197988

m=3(γ)

Charge = -1 Multiplicity = 2

C	4.777334	-0.405792	-0.05396
C	3.492718	0.44841	0.02721
C	2.201511	-0.403869	0.088942
C	0.938827	0.40595	-0.299576
C	-0.382504	-0.222191	0.192656
C	-1.61008	0.332521	-0.474154
C	-2.893004	-0.272207	0.059423
H	-2.869755	-1.351614	-0.103586
H	-2.966732	-0.097588	1.132629
C	-4.094933	0.32617	-0.65192
H	-4.147155	1.406101	-0.515952
H	-4.081686	0.105013	-1.718338
F	4.915499	-0.927493	-1.261997
F	4.730421	-1.384091	0.841142
F	5.82514	0.36254	0.201714
F	3.457689	1.243678	-1.049866
F	3.568474	1.202953	1.127356
F	2.330421	-1.437681	-0.755038
F	2.073624	-0.879552	1.333538
F	0.914066	0.499622	-1.63785
F	1.04631	1.642231	0.213437
F	-0.283939	-1.561271	-0.025279
F	-0.439577	-0.045521	1.532829

H	-1.604033	1.494273	-0.240706
H	-1.520967	0.266475	-1.557057
O	-1.764804	2.773107	0.239885
H	-2.571416	2.60784	0.758526
S	-5.636345	-0.320412	-0.02719
O	-5.678949	0.023737	1.403126
O	-5.602467	-1.773648	-0.255658
O	-6.688668	0.352228	-0.803863

m=4(α)

Charge = -1 Multiplicity = 2

C	4.854204	-0.029414	0.397181
C	3.58087	-0.055889	-0.474692
C	2.280634	-0.23768	0.345391
C	1.00169	0.200454	-0.396927
C	-0.263976	-0.314439	0.226648
C	-1.500625	0.250416	-0.46562
C	-2.767615	-0.382825	0.100768
C	-3.999993	0.164932	-0.574335
H	-4.008803	0.052174	-1.657978
H	-4.064803	1.318983	-0.370277
F	4.947174	1.114498	1.057172
F	4.83562	-1.032761	1.265649
F	3.54064	1.089545	-1.167449
F	3.697961	-1.076945	-1.332006
F	2.382235	0.470036	1.484366
F	2.188014	-1.537938	0.667549
F	1.017673	1.556822	-0.43732
F	1.128515	-0.227747	-1.682673
S	-5.542024	-0.444675	0.080914
O	-5.481595	-1.908848	-0.017165
O	-5.589646	0.032123	1.474755
O	-6.594077	0.14721	-0.753801
F	5.918117	-0.156776	-0.382898
H	-2.826753	-0.203714	1.175931
H	-2.734146	-1.464681	-0.049759
H	-1.540872	1.33173	-0.330369
H	-1.446604	0.054194	-1.537696
H	-0.253446	-0.045349	1.284086
H	-0.247252	-1.401619	0.153731
O	-4.267361	2.490065	0.388945

H	-4.758181	2.026747	1.09384

m=4(β)

Charge = -1 Multiplicity = 2

C	-4.597059	-0.026703	-0.004577
C	-3.169217	-0.377617	-0.475429
C	-2.071284	0.414384	0.27599
C	-0.670741	-0.22611	0.205242
C	0.43529	0.695918	0.632533
C	1.787079	-0.011477	0.635451
C	2.881683	0.956841	1.037639
C	4.276409	0.391596	1.20059
H	4.320554	-0.301471	2.042088
H	4.995894	1.189781	1.373491
F	-4.843518	-0.568545	1.177985
F	-4.740484	1.289768	0.081227
F	-2.998574	-1.694882	-0.305849
F	-3.088719	-0.095795	-1.781123
F	-2.427631	0.532419	1.567431
F	-2.027555	1.644548	-0.26057
F	-0.708909	-1.339918	0.979391
F	-0.499398	-0.648551	-1.076734
S	4.909844	-0.536577	-0.194861
O	4.202082	-1.823307	-0.216763
O	4.634612	0.268504	-1.403904
O	6.348314	-0.684715	0.059885
F	-5.474154	-0.497542	-0.87941
H	2.616154	1.496023	1.949086
H	2.912809	1.796716	0.242356
H	1.774561	-0.847766	1.338275
H	1.994013	-0.421854	-0.352881
H	0.192611	1.070943	1.628087
H	0.449817	1.541674	-0.055132
O	3.130368	2.576579	-0.974643
H	3.710584	1.870179	-1.329953

m=4(γ)

Charge = -1 Multiplicity = 2

C	4.731828	-0.472694	0.080048
C	3.457504	0.387918	-0.056112
C	2.157013	-0.395411	0.247577
C	0.880684	0.253297	-0.324182

C	-0.388129	-0.318325	0.244687
C	-1.62239	0.276251	-0.409058
C	-2.907362	-0.337928	0.112289
H	-2.877654	-1.415731	-0.062999
H	-2.973113	-0.183607	1.190669
C	-4.122712	0.258177	-0.577315
H	-4.179652	1.337743	-0.436705
H	-4.122269	0.04434	-1.645638
F	4.704662	-1.152679	1.219229
F	4.834427	-1.321243	-0.930892
F	5.794213	0.319897	0.077556
F	3.559657	1.406096	0.806559
F	3.431496	0.876755	-1.302356
F	2.049963	-0.491577	1.582419
F	2.268743	-1.637031	-0.255785
F	0.976848	1.588226	-0.087962
F	0.926927	0.091559	-1.670174
H	-1.636398	1.404003	-0.159564
H	-1.56994	0.236513	-1.497786
H	-0.396298	-0.135912	1.318811
H	-0.36565	-1.398909	0.083842
O	-1.799336	2.725383	0.478054
H	-2.672173	2.534966	0.862724
S	-5.658005	-0.392689	0.054901
O	-5.697803	-0.048461	1.486122
O	-6.719881	0.27406	-0.715739
O	-5.622957	-1.846996	-0.171776

m=4(δ)

Charge = -1 Multiplicity = 2

C	-4.662486	0.309896	0.05566
C	-3.397764	-0.573473	0.118291
C	-2.084637	0.243261	0.173161
C	-0.832456	-0.561415	-0.235986
C	0.462643	0.057343	0.208377
C	1.682899	-0.607241	-0.391451
C	2.972529	0.018283	0.129699
H	2.996387	1.076948	-0.133328
H	2.998898	-0.05321	1.217867
C	4.18556	-0.679038	-0.461661
H	4.209418	-1.73668	-0.200098

H	4.21364	-0.585239	-1.546971
F	-4.590521	1.276092	0.962596
F	-4.797959	0.850457	-1.144981
F	-5.727596	-0.437232	0.307809
F	-3.485084	-1.331242	1.217482
F	-3.40247	-1.367935	-0.959959
F	-1.93713	0.695051	1.428135
F	-2.200639	1.302188	-0.645648
F	-0.967147	-1.807847	0.29332
F	-0.876064	-0.703061	-1.58124
H	1.661764	-1.670366	-0.133335
H	1.646626	-0.538582	-1.479248
H	0.490479	0.105981	1.295481
H	0.424773	1.181802	-0.151871
O	0.53769	2.526923	-0.459938
H	1.345498	2.699426	0.054631
S	5.72573	0.001025	0.126366
O	5.729545	1.423707	-0.25506
O	5.736086	-0.187888	1.586851
O	6.784753	-0.766542	-0.549249

(3-4) Formula: $F\text{-}(CF_2)_{8-m}\text{-}(CH_2)_m\text{-}PO_4^{2-}$

m=2(α)

Charge = -2 Multiplicity = 2

C	-5.34459	-0.324169	0.144217
C	-4.039852	0.488653	-0.012321
C	-2.786817	-0.408373	-0.160831
C	-1.472636	0.355162	0.141417
C	-0.227172	-0.352142	-0.451517
C	1.106226	0.075931	0.197591
C	2.314773	-0.340891	-0.593113
H	2.262369	0.111035	-1.582545
H	2.286093	-1.426111	-0.703129
C	3.605531	0.066052	0.095014
H	3.651701	-0.276919	1.13171
H	3.660546	1.205388	0.143683
F	-6.381144	0.479263	-0.035678
F	-5.384952	-1.292273	-0.762083
F	-5.420001	-0.855202	1.353409
F	-3.905418	1.2715	1.065156
F	-4.158068	1.254577	-1.100224
F	-2.749995	-0.87562	-1.415102
F	-2.8919	-1.441171	0.68518
F	-1.345756	0.463647	1.469013
F	-1.564788	1.584248	-0.386629
F	-0.189768	-0.07513	-1.7637
F	-0.373251	-1.679354	-0.29791
F	1.13262	-0.458608	1.442684
F	1.048794	1.426353	0.354257
O	4.68034	-0.404112	-0.660105
P	6.18476	-0.415853	0.097757
O	6.043897	-1.417968	1.232117
O	7.085828	-0.862364	-1.03699
O	6.396714	1.012926	0.567678
O	3.694834	2.717291	-0.266017
H	2.874849	2.67681	-0.787632

m=2(β)

Charge = -2 Multiplicity = 2

C	5.299014	0.096621	0.139997

C	3.967908	-0.568413	-0.275073
C	2.733502	0.329817	-0.015652
C	1.412226	-0.480306	0.008087
C	0.164	0.410789	-0.212568
C	-1.152636	-0.241135	0.266995
C	-2.391527	0.374052	-0.316796
H	-2.399446	0.252641	-1.397472
H	-2.350523	1.53432	-0.119316
C	-3.657459	-0.138255	0.331184
H	-3.687119	0.135139	1.387485
H	-3.673565	-1.231604	0.259758
F	6.305561	-0.59376	-0.37268
F	5.346639	1.338898	-0.323129
F	5.421247	0.116722	1.456934
F	3.840878	-1.710368	0.412131
F	4.036849	-0.844917	-1.579818
F	2.671173	1.252235	-0.983871
F	2.885572	0.946447	1.163327
F	1.318794	-1.094583	1.193828
F	1.463669	-1.405546	-0.960168
F	0.073522	0.6821	-1.522652
F	0.34469	1.564395	0.452174
F	-1.161256	-0.179002	1.618388
F	-1.082786	-1.558935	-0.066342
O	-4.756844	0.421519	-0.357512
P	-6.238004	-0.3037	-0.077505
O	-6.440358	-0.24363	1.430258
O	-7.173743	0.581856	-0.879501
O	-6.098746	-1.723042	-0.609125
O	-2.303974	2.895223	0.111956
H	-1.56108	3.087387	-0.486609

m=3(α)

Charge = -2 Multiplicity = 2

C	-5.051954	-0.543245	0.076419
C	-3.82808	0.393192	-0.024836
C	-2.481553	-0.366891	-0.105835
C	-1.274042	0.528143	0.268023
C	0.085596	0.003424	-0.240282
C	1.261528	0.672079	0.412039
C	2.582685	0.21504	-0.19684

H	2.629022	0.468939	-1.256267
H	2.688295	-0.86753	-0.103399
C	3.731586	0.888365	0.524734
H	3.738101	0.657094	1.592979
H	3.553333	2.016573	0.46747
F	-6.152793	0.158484	-0.148791
F	-4.963321	-1.509302	-0.828424
F	-5.129643	-1.081946	1.282499
F	-3.832642	1.19013	1.051713
F	-3.972325	1.140113	-1.123862
F	-2.338818	-0.830344	-1.35359
F	-2.525929	-1.409255	0.736825
F	-1.241846	0.625349	1.606448
F	-1.477854	1.756012	-0.241403
O	4.9902	0.677493	-0.055024
P	5.697273	-0.842579	0.039839
O	5.129848	-1.632509	-1.130005
O	7.171199	-0.505526	-0.102431
O	5.292716	-1.389653	1.400068
H	1.137571	1.750561	0.297333
H	1.227425	0.438364	1.475888
O	3.467223	3.397267	-0.199092
H	3.978848	3.107067	-0.973722
F	0.094351	-1.340016	-0.028499
F	0.099068	0.184153	-1.58475

m=3(β)

Charge = -2 Multiplicity = 2

C	-5.208077	-0.289983	-0.205488
C	-3.902795	0.071723	0.537319
C	-2.643066	-0.049446	-0.354595
C	-1.337815	-0.153187	0.471952
C	-0.059621	0.188432	-0.323675
C	1.202172	-0.267025	0.353867
C	2.442062	0.188362	-0.391191
H	2.536414	1.334223	-0.313484
H	2.391366	-0.025923	-1.459282
C	3.69948	-0.37365	0.224238
H	3.65875	-1.467266	0.187893
H	3.768187	-0.071781	1.273729
F	-6.24346	0.111773	0.515964

F	-5.243534	0.314498	-1.385882
F	-5.294786	-1.598317	-0.383009
F	-3.790277	-0.747165	1.590945
F	-4.009204	1.331376	0.97019
F	-2.591504	1.02454	-1.152338
F	-2.761296	-1.146222	-1.116832
F	-1.24918	-1.408825	0.936814
F	-1.426853	0.683883	1.520089
F	-0.060101	1.534265	-0.511305
F	-0.191525	-0.371607	-1.553537
O	4.818816	0.099667	-0.502729
P	6.318133	-0.383112	0.040963
O	6.282871	-1.905715	0.044262
O	7.240747	0.223028	-1.002973
O	6.464926	0.217393	1.433648
H	1.200043	0.115471	1.375877
H	1.174401	-1.356674	0.401609
O	2.622442	2.732831	0.141857
H	1.661873	2.835862	0.252221

m=3(γ)

Charge = -2 Multiplicity = 2

C	4.897066	-0.712213	-0.13308
C	3.727329	0.279306	0.051784
C	2.342091	-0.412244	0.080252
C	1.181915	0.572935	-0.207233
C	-0.199893	0.061901	0.264201
C	-1.367481	0.754002	-0.378064
C	-2.706635	0.311065	0.171722
H	-2.769234	0.521546	1.23985
H	-2.811068	-0.768157	0.036603
C	-3.825304	1.036711	-0.563467
H	-3.823843	0.742935	-1.615291
H	-3.651335	2.112189	-0.512168
F	6.035354	-0.094306	0.143998
F	4.755234	-1.743874	0.688677
F	4.943258	-1.151109	-1.380471
F	3.772947	1.159118	-0.956784
F	3.915105	0.925148	1.206309
F	2.177252	-0.962212	1.290031
F	2.329932	-1.384403	-0.842489

F	1.149425	0.79504	-1.529489
F	1.455233	1.732995	0.414284
F	-0.232663	0.195497	1.610859
F	-0.237087	-1.272388	0.000587
O	-5.106157	0.815709	0.00336
P	-5.771609	-0.711346	-0.025701
O	-5.203769	-1.442907	1.184368
O	-7.257701	-0.407534	0.089886
O	-5.349999	-1.324197	-1.354613
H	-1.249209	1.902175	-0.153876
H	-1.299031	0.67423	-1.461949
O	-1.081937	3.259342	0.117387
H	-0.696071	3.13765	1.002943

m=4(α)

Charge = -2 Multiplicity = 2

C	-5.032687	-0.588265	-0.034692
C	-3.815845	0.360686	-0.034291
C	-2.465191	-0.374946	-0.214491
C	-1.241089	0.435028	0.25783
C	0.070861	-0.103518	-0.237605
C	1.250763	0.651365	0.366941
C	2.571644	0.152827	-0.206336
H	2.603018	0.314329	-1.286209
H	2.672762	-0.92183	-0.032391
C	3.739075	0.868116	0.436799
H	3.773066	0.709884	1.518022
H	3.558435	1.988222	0.308162
F	-6.142347	0.12586	-0.160011
F	-4.950125	-1.436732	-1.051719
F	-5.094068	-1.271187	1.097892
F	-3.831284	1.036511	1.121778
F	-3.974983	1.225338	-1.043544
F	-2.336168	-0.663458	-1.519621
F	-2.505754	-1.533008	0.468187
F	-1.286878	0.45358	1.614292
F	-1.43764	1.717396	-0.154753
O	4.990211	0.623437	-0.152894
P	5.679282	-0.899279	-0.023652
O	5.098556	-1.715113	-1.169565
O	7.157328	-0.584116	-0.181669

O	5.278182	-1.409381	1.352392
H	1.147048	1.719108	0.164087
H	1.251238	0.52344	1.450357
H	0.074073	-0.017003	-1.323881
H	0.116972	-1.163515	0.017844
O	3.583243	3.334896	-0.449327
H	4.322043	3.042294	-1.010158

m=4(β)

Charge = -2 Multiplicity = 2

C	5.135796	0.288229	-0.157776
C	3.800065	-0.057779	0.533887
C	2.561925	0.197657	-0.359116
C	1.291319	-0.549154	0.095782
C	0.03012	-0.041896	-0.543598
C	-1.182322	-0.866586	-0.121424
C	-2.452745	-0.328194	-0.745232
H	-2.392385	-0.284926	-1.834562
H	-2.568654	0.77901	-0.41595
C	-3.694891	-1.055922	-0.292641
H	-3.761873	-1.032044	0.797489
H	-3.639054	-2.104567	-0.597677
F	6.101728	0.304821	0.749988
F	5.435237	-0.613827	-1.079304
F	5.060067	1.484348	-0.727228
F	3.705856	0.701021	1.632273
F	3.855623	-1.344995	0.899017
F	2.852759	-0.172586	-1.618769
F	2.329748	1.520258	-0.353048
F	1.239134	-0.442391	1.451245
F	1.487579	-1.863074	-0.181854
O	-4.851975	-0.473681	-0.884906
P	-6.009223	0.124679	0.137188
O	-5.293919	1.194941	0.973512
O	-7.039782	0.681002	-0.824886
O	-6.482106	-1.04319	0.987067
H	-1.048483	-1.907176	-0.426002
H	-1.278018	-0.855407	0.965774
H	0.166628	-0.077227	-1.625614
H	-0.097089	1.000195	-0.251097
O	-2.948244	2.043303	0.180897

H	-3.85972	1.712663	0.466169

m=4(γ)

Charge = -2 Multiplicity = 2

C	-4.883179	-0.718548	-0.059188
C	-3.698299	0.262086	0.072046
C	-2.328434	-0.385042	-0.24743
C	-1.119167	0.396764	0.305306
C	0.197588	-0.035391	-0.277992
C	1.367717	0.708402	0.339963
C	2.706736	0.255197	-0.204815
H	2.737165	0.399144	-1.287272
H	2.825097	-0.814469	-0.013653
C	3.84159	1.028411	0.44756
H	3.873661	0.804104	1.516233
H	3.661542	2.098446	0.333747
F	-6.017483	-0.032964	-0.041166
F	-4.801297	-1.384529	-1.203811
F	-4.893434	-1.580242	0.945846
F	-3.708701	0.74391	1.321435
F	-3.910551	1.26957	-0.783023
F	-2.229288	-0.47457	-1.583359
F	-2.306792	-1.629528	0.260725
F	-1.130923	0.241288	1.652039
F	-1.362455	1.714016	0.063538
O	5.113936	0.781344	-0.13569
P	5.784524	-0.738639	-0.046321
O	5.207988	-1.528548	-1.215309
O	7.269339	-0.437467	-0.191952
O	5.382806	-1.294128	1.31422
H	1.268403	1.829334	0.087201
H	1.341187	0.673776	1.430425
O	1.195851	3.141955	-0.608046
H	0.439773	2.892176	-1.166412
H	0.16586	0.126328	-1.355118
H	0.301096	-1.108322	-0.098836

(4-1) Formula: $(CF_3)_2$-CH-CF_2-CH_2-X

X=-OH (α)
Charge =0 Multiplicity = 2

C	1.815736	-0.567263	0.108478
C	0.534065	-0.078336	-0.573277
C	-0.68057	-0.92013	-0.159476
C	0.34926	1.411861	-0.311147
F	1.871005	-1.894412	0.178179
F	1.92716	-0.097489	1.354515
F	2.891835	-0.160504	-0.566547
F	1.486497	2.079592	-0.507618
F	-0.048795	1.66072	0.937348
F	-0.564064	1.927265	-1.13589
H	0.668615	-0.200664	-1.648673
C	-2.039384	-0.414525	-0.604598
H	-2.291197	0.560837	-0.029219
H	-2.028645	-0.151321	-1.662579
F	-0.677659	-1.08203	1.19333
F	-0.509111	-2.160698	-0.686728
O	-2.936077	1.49893	0.88261
H	-2.550246	1.127594	1.6953
O	-2.976091	-1.390509	-0.282742
H	-3.767637	-1.245459	-0.812957

X=-OH (γ)
Charge =0 Multiplicity = 2

C	-1.290606	-1.015222	-0.201273
C	-0.250752	0.006862	0.247805
C	1.189908	-0.445841	0.000293
C	-0.579083	1.395701	-0.275481
F	-0.876585	-2.261244	-0.000563
F	-1.557695	-0.880227	-1.505098
F	-2.437066	-0.859549	0.458622
F	-1.885346	1.642713	-0.204058
F	-0.210644	1.531698	-1.55284
F	0.048718	2.337129	0.426659
H	-0.352726	0.068486	1.476067
C	2.271505	0.607241	0.166133
H	2.117148	1.409461	-0.554061

H	2.205914	1.004692	1.177552
O	3.535969	0.007974	0.006219
H	3.716553	-0.088839	-0.934993
F	1.257514	-0.971076	-1.259514
F	1.448639	-1.475092	0.846681
O	-0.594234	0.229103	2.702803
H	-1.354427	0.83798	2.64941

X=-COO^- (α)

Charge = -1 Multiplicity = 2

C	1.989558	-0.949609	0.146187
C	0.883644	-0.162288	-0.562865
C	-0.516465	-0.603692	-0.105271
C	1.126572	1.331602	-0.380227
F	1.671401	-2.230696	0.310975
F	2.261135	-0.449214	1.356007
F	3.120759	-0.911237	-0.560709
F	2.407296	1.639784	-0.595921
F	0.818908	1.747814	0.848273
F	0.396893	2.044933	-1.239348
H	0.964614	-0.374744	-1.629382
C	-1.680828	0.229606	-0.582132
H	-1.653037	1.274937	0.004375
H	-1.586334	0.461797	-1.63975
F	-0.524124	-0.691221	1.255815
F	-0.694256	-1.879161	-0.557059
O	-2.042657	2.202143	0.886088
H	-2.748291	1.620024	1.235903
C	-3.033288	-0.422886	-0.245832
O	-3.53551	-0.155339	0.870996
O	-3.511112	-1.166484	-1.12616

X=-COO^- (γ)

Charge = -1 Multiplicity = 2

C	-1.678312	-1.008875	-0.22333
C	-0.681811	0.004251	0.28226
C	0.735883	-0.35467	-0.109688
C	-1.080683	1.386888	-0.152805
F	-1.209232	-2.258441	-0.144158
F	-2.041722	-0.817745	-1.507941
F	-2.813223	-0.979415	0.490761

F	-2.400806	1.577528	-0.038334
F	-0.765415	1.672672	-1.432892
F	-0.487249	2.330682	0.593013
H	-0.709935	-0.024542	1.52522
C	1.772723	0.729619	0.133927
H	1.628988	1.5665	-0.547076
H	1.693766	1.068326	1.165987
F	0.802536	-0.756077	-1.419883
F	1.119606	-1.454254	0.611414
O	-0.705185	-0.07787	2.931865
H	0.185851	-0.375388	3.137639
C	3.147868	0.170141	-0.136151
O	3.824499	-0.058541	0.977373
O	3.639045	-0.067786	-1.211094

X=-SO_3^- (α)

Charge =-1 Multiplicity = 2

C	2.353918	-1.03633	0.050285
C	1.242747	-0.16463	-0.548053
C	-0.140127	-0.513965	0.032421
C	1.615441	1.307231	-0.387498
F	1.975266	-2.300028	0.21599
F	2.756661	-0.583068	1.241565
F	3.420967	-1.04684	-0.750982
F	2.878756	1.520322	-0.759969
F	1.498413	1.729576	0.873185
F	0.842672	2.085144	-1.145424
H	1.208064	-0.372298	-1.618436
C	-1.278562	0.380604	-0.409307
H	-1.293458	1.389319	0.242067
H	-1.180104	0.700258	-1.443891
F	-0.04693	-0.543773	1.38973
F	-0.42107	-1.787818	-0.351073
O	-1.369166	2.440048	1.04462
H	-0.860379	2.095629	1.799157
S	-2.934954	-0.292134	-0.178064
O	-3.091823	-1.299106	-1.22724
O	-3.800266	0.871861	-0.364605
O	-2.965991	-0.842535	1.175457

X=-SO_3^- (γ)

Charge =-1 Multiplicity = 2

C	-2.18508	-0.95323	-0.242396
C	-1.116105	0.01535	0.255487
C	0.30825	-0.393636	-0.148138
C	-1.482355	1.453978	-0.082561
F	-1.763795	-2.212658	-0.226441
F	-2.539961	-0.660405	-1.498873
F	-3.283636	-0.887983	0.507792
F	-2.788635	1.666365	0.060543
F	-1.162024	1.750785	-1.345541
F	-0.844698	2.314338	0.70778
H	-1.140444	-0.023352	1.486494
C	1.370663	0.643861	0.126899
H	1.276866	1.464065	-0.58113
H	1.268432	1.018343	1.143446
F	0.272109	-0.706358	-1.475064
F	0.599448	-1.547358	0.50408
S	3.062048	0.026634	-0.014864
O	3.130001	-0.727307	-1.267507
O	3.297647	-0.797732	1.172188
O	3.862591	1.25379	-0.028373
O	-1.15128	-0.199767	2.732422
H	-1.280809	-1.16553	2.754947

X=-PO_4^{2-} (α)

Charge =-2 Multiplicity = 2

C	-2.864883	-0.859561	0.011702
C	-1.618446	-0.151917	0.547728
C	-0.334576	-0.742638	-0.050284
C	-1.743012	1.350056	0.319575
F	-2.680454	-2.171079	-0.113784
F	-3.225091	-0.390192	-1.187352
F	-3.89983	-0.681274	0.834329
F	-2.965318	1.787212	0.626985
F	-1.506229	1.688765	-0.949009
F	-0.877455	2.017684	1.083318
H	-1.587919	-0.314593	1.625454
C	0.944175	0.026794	0.215897
H	0.878435	1.052518	-0.356017
H	1.037808	0.265193	1.277543
F	-0.498665	-0.90966	-1.392209

F	-0.186593	-1.993179	0.464682
O	1.36433	2.191496	-1.057135
H	2.310069	1.903795	-0.898519
O	1.999653	-0.710537	-0.281657
P	3.560851	-0.236458	0.168003
O	3.542291	-0.210781	1.68077
O	3.720351	1.144439	-0.466683
O	4.399126	-1.318483	-0.467653

X=-PO_4^{2-} (γ)

Charge =-2 Multiplicity = 2

C	-2.585941	-0.940553	0.004725
C	-1.412275	0.008189	0.230584
C	-0.080782	-0.54308	-0.284528
C	-1.746304	1.414829	-0.240103
F	-2.224268	-2.213262	0.117072
F	-3.106639	-0.77265	-1.216026
F	-3.558913	-0.718845	0.887568
F	-2.99821	1.743363	0.073727
F	-1.621052	1.525924	-1.566087
F	-0.94095	2.316629	0.317226
H	-1.308021	0.086237	1.457169
C	1.079327	0.430067	-0.315523
H	0.8484	1.254876	-0.990347
H	1.210893	0.817351	0.697733
F	-0.294694	-1.050966	-1.535086
F	0.257926	-1.602457	0.494146
O	-1.090772	0.279244	2.683788
H	-0.225205	0.725378	2.633893
O	2.205143	-0.275873	-0.771138
P	3.638746	0.010103	0.055309
O	3.389684	-0.495005	1.467484
O	3.842338	1.515812	-0.02062
O	4.62233	-0.811894	-0.753498

(4-2) Formula: $(CF_3)_2$-CH-CF(CF_3)-CH_2-X

X=-OH (α)

Charge =0 Multiplicity = 2

C	1.907716	-0.767763	-0.506661
C	0.698765	0.168014	-0.572254
C	-0.648967	-0.587194	-0.379311
C	0.964563	1.392897	0.315309
F	1.947004	-1.591337	-1.550497
F	1.924231	-1.507459	0.602116
F	3.040319	-0.055781	-0.532004
F	1.666191	2.302449	-0.36246
F	1.664389	1.103275	1.414497
F	-0.167394	1.974171	0.70776
H	0.69388	0.551598	-1.594338
C	-1.672555	-0.094695	-1.387634
H	-1.769531	1.058686	-1.31275
H	-1.280802	-0.272161	-2.390782
O	-2.891849	-0.716877	-1.155647
H	-3.407038	-0.713169	-1.970008
F	-0.410307	-1.916647	-0.669591
C	-1.238604	-0.611169	1.058181
F	-0.27772	-0.533432	1.981312
F	-2.088622	0.390438	1.267741
F	-1.897583	-1.745078	1.264457
O	-2.168082	2.469943	-1.410661
H	-2.427153	2.564585	-0.477424

X=-OH (γ)

Charge =0 Multiplicity = 2

C	-1.519084	-0.772485	-0.826799
C	-0.643446	-0.159864	0.267383
C	0.851452	-0.520459	0.162668
C	-1.017916	1.298112	0.53416
F	-1.631546	-2.088823	-0.675225
F	-1.039092	-0.544118	-2.048378
F	-2.750764	-0.260156	-0.778329
F	-2.164353	1.373699	1.206695
F	-1.17475	1.992781	-0.594376
F	-0.086847	1.908377	1.263949

H	-1.072147	-0.695349	1.28119
C	1.472404	-0.740859	1.544562
H	1.296311	0.134938	2.165117
H	0.959899	-1.597275	1.98391
O	2.861344	-0.949727	1.467045
H	3.026032	-1.838084	1.131899
F	0.923597	-1.712871	-0.530229
C	1.719181	0.464687	-0.670339
F	1.034683	1.02061	-1.671227
F	2.194348	1.449824	0.086623
F	2.749504	-0.176894	-1.207885
O	-1.681884	-1.287367	2.252264
H	-1.314331	-2.184131	2.149029

X=-COO^- (α)

Charge = -1 Multiplicity = 2

C	2.140847	-0.748252	-0.719124
C	0.958357	0.214291	-0.611121
C	-0.395125	-0.495984	-0.301606
C	1.325294	1.404835	0.286459
F	2.05858	-1.498423	-1.815774
F	2.242818	-1.568849	0.326334
F	3.286185	-0.061003	-0.808455
F	1.87584	2.378269	-0.441015
F	2.201597	1.099793	1.245896
F	0.244597	1.912082	0.882266
H	0.851777	0.62881	-1.614056
C	-1.53171	0.232673	-1.000025
H	-1.491389	1.407745	-0.732401
H	-1.3335	0.212906	-2.072041
F	-0.286648	-1.754303	-0.858671
C	-0.687618	-0.736876	1.215401
F	0.396084	-0.548013	1.974554
F	-1.626983	0.098555	1.661217
F	-1.098385	-1.976672	1.437972
O	-1.982988	2.646612	-0.696686
H	-2.898642	2.307158	-0.789981
C	-2.969205	-0.228026	-0.731741
O	-3.863471	0.644596	-0.846342
O	-3.130595	-1.434399	-0.464458

X=-COO^- (γ)

Charge = -1 Multiplicity = 2

C	1.86026	0.78069	-0.787965
C	0.88428	0.252697	0.270833
C	-0.60764	0.316295	-0.14227
C	1.376257	-1.034801	0.927227
F	1.73917	2.099108	-0.926165
F	1.672199	0.231482	-1.985975
F	3.124018	0.53645	-0.437708
F	2.508534	-0.832223	1.596098
F	1.606082	-1.990967	0.022188
F	0.489001	-1.503471	1.801425
H	1.036905	1.049719	1.185265
C	-1.499713	0.675801	1.040944
H	-1.32253	-0.034787	1.843433
H	-1.180889	1.663695	1.369409
F	-0.702418	1.297793	-1.108642
C	-1.120774	-0.953596	-0.865852
F	-0.288495	-1.373827	-1.815289
F	-1.307631	-1.95703	-0.012543
F	-2.284224	-0.688087	-1.455009
O	1.392377	1.944221	2.042915
H	0.914469	2.70913	1.672621
C	-3.004559	0.729874	0.710383
O	-3.710098	-0.218752	1.124732
O	-3.405123	1.729212	0.070358

X=-SO_3^- (α)

Charge =-1 Multiplicity = 2

C	2.390473	-0.829834	-0.859542
C	1.278005	0.199866	-0.61038
C	-0.059726	-0.454193	-0.130782
C	1.790621	1.373231	0.224739
F	2.133106	-1.53193	-1.962101
F	2.557687	-1.692313	0.139413
F	3.564065	-0.220678	-1.049216
F	2.680382	2.08927	-0.460663
F	2.380484	0.980112	1.3562
F	0.797045	2.198735	0.548006
H	1.079035	0.629717	-1.593977

C	-1.229287	0.250623	-0.801559
H	-1.196445	1.454347	-0.617974
H	-1.108119	0.141353	-1.8782
F	-0.043781	-1.756238	-0.595344
C	-0.220929	-0.622495	1.397446
F	0.882986	-1.109978	1.959771
F	-0.507707	0.529934	1.992678
F	-1.197046	-1.486303	1.64821
O	-1.565283	2.699969	-0.766098
H	-2.434071	2.524982	-1.173808
S	-2.948798	-0.155524	-0.433566
O	-3.223226	0.284633	0.930189
O	-3.653226	0.641443	-1.443271
O	-3.06821	-1.597381	-0.634707

X=-SO_3^- (γ)

Charge =-1 Multiplicity = 2

C	2.222046	0.240572	-1.112552
C	1.189881	0.405447	0.011547
C	-0.243512	-0.063342	-0.357447
C	1.735769	0.000422	1.379045
F	1.994209	1.128219	-2.078799
F	2.21523	-0.968426	-1.665822
F	3.456094	0.458124	-0.656253
F	2.737289	0.789177	1.756292
F	2.192822	-1.254619	1.3748
F	0.794879	0.089891	2.317743
H	1.143739	1.627911	0.076443
C	-1.26649	0.888839	0.254417
H	-1.118602	0.974518	1.328395
H	-1.08896	1.862247	-0.199111
F	-0.327327	0.003098	-1.730456
C	-0.512048	-1.555869	-0.036274
F	0.508506	-2.332678	-0.396626
F	-0.720096	-1.739803	1.263644
F	-1.575481	-1.976737	-0.705772
O	1.288919	2.89649	0.226077
H	0.914585	2.987368	1.121647
S	-3.031017	0.577929	0.016908
O	-3.386004	-0.551763	0.87705
O	-3.624405	1.841736	0.463554

O	-3.227697	0.318348	-1.409064

X=-PO_4^{2-} (α)

Charge =-2 Multiplicity = 2

C	2.535966	1.064144	-0.629334
C	1.45024	0.543972	0.317402
C	0.238021	-0.071458	-0.434691
C	2.074811	-0.29978	1.430032
F	2.141206	2.182834	-1.23406
F	2.872363	0.189142	-1.575394
F	3.649325	1.358007	0.050799
F	2.657485	0.486776	2.335467
F	3.007762	-1.143438	0.983823
F	1.152107	-1.01898	2.069095
H	1.069883	1.433536	0.824623
C	-1.040536	0.250738	0.320362
H	-0.975067	-0.040216	1.370886
H	-1.079811	1.417733	0.318384
F	0.177459	0.548202	-1.666307
C	0.30794	-1.585896	-0.767796
F	1.54991	-1.99287	-1.032842
F	-0.15185	-2.324904	0.239483
F	-0.429341	-1.852852	-1.839698
O	-2.131239	-0.28095	-0.334834
P	-3.665569	0.127299	0.251485
O	-3.824396	1.594114	-0.145137
O	-3.582762	-0.089869	1.747182
O	-4.547596	-0.825474	-0.516395
O	-1.492902	2.790713	0.16054
H	-2.436806	2.473619	0.033832

X=-PO_4^{2-} (γ)

Charge =-2 Multiplicity = 2

C	-2.609407	-0.255824	-0.966785
C	-1.419163	-0.441958	-0.02588
C	-0.115303	0.226744	-0.508664
C	-1.8337	-0.256865	1.434786
F	-2.443133	-0.924591	-2.103916
F	-2.81331	1.024661	-1.275071
F	-3.727318	-0.714396	-0.397591
F	-2.47591	-1.334973	1.881382
F	-2.652109	0.783946	1.602297

F	-0.771854	-0.070704	2.215316
H	-1.233203	-1.653702	-0.068054
C	1.099237	-0.640456	-0.205531
H	1.127937	-0.854287	0.865785
H	0.963688	-1.577683	-0.748708
F	-0.223252	0.354941	-1.878361
C	0.113339	1.679382	0.004302
F	-1.04005	2.315649	0.229717
F	0.80547	1.694969	1.139246
F	0.782102	2.387695	-0.896438
O	-1.251882	-2.935319	-0.190998
H	-0.875223	-3.023196	-1.08573
O	2.246507	0.038143	-0.642397
P	3.69676	-0.477758	0.032066
O	3.598962	-0.112357	1.50429
O	3.726983	-1.977414	-0.220753
O	4.703135	0.331235	-0.761003

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(4-3) Formula: $(CF_3)_2$-CH-CH_2-X

X=-OH (α)

Charge =0 Multiplicity = 2

C	0.440321	1.198211	-0.106585
C	-0.132429	-0.092574	-0.672882
H	-0.350804	0.092182	-1.725947
C	0.82757	-1.273107	-0.56857
H	1.362031	-1.245311	0.446936
H	0.283772	-2.218229	-0.584696
C	-1.448751	-0.430574	0.000592
F	-0.204687	2.269793	-0.577323
F	0.353775	1.249864	1.230338
F	1.727298	1.339601	-0.424018
F	-2.239279	0.6384	0.133747
F	-1.269617	-0.94451	1.224381
F	-2.121441	-1.338462	-0.710341
O	1.769863	-1.190534	-1.597061
H	2.237821	-2.031303	-1.6504
O	2.082801	-1.190098	1.774408
H	1.311164	-0.896191	2.288942

X=-OH (β)

Charge =0 Multiplicity = 2

C	1.422053	0.276359	-0.015503
C	-0.091317	0.276544	-0.036338
H	-0.423143	0.786106	1.01563
C	-0.640672	1.144956	-1.154294
H	0.044332	1.975505	-1.326297
H	-0.702906	0.550686	-2.070441
C	-0.665756	-1.125227	0.010757
F	1.921026	-0.614763	0.842861
F	1.923185	-0.011547	-1.223966
F	1.890254	1.476178	0.330201
F	-0.499301	-1.698806	1.204781
F	-0.077426	-1.920913	-0.894567
F	-1.97094	-1.122806	-0.251614
O	-1.916337	1.618196	-0.764233
H	-2.249004	2.190316	-1.464144
O	-1.055512	1.413324	1.959016

H	-1.721525	1.84334	1.389985

X=COO$^-$ (α)

Charge = -1 Multiplicity = 2

C	0.329524	-1.314949	-0.06474
C	0.345879	0.138473	-0.511162
H	0.327796	0.131729	-1.602856
C	-0.857992	0.90381	0.0076
H	-0.988058	0.687949	1.165323
H	-0.693048	1.980046	-0.045472
C	1.636785	0.816163	-0.096029
F	1.152091	-2.073833	-0.794596
F	0.696134	-1.459289	1.215218
F	-0.895834	-1.835461	-0.184407
F	2.715043	0.07441	-0.372152
F	1.671736	1.086145	1.214481
F	1.779408	1.979166	-0.738392
O	-1.632844	0.378134	2.330013
H	-2.487137	0.340349	1.850425
C	-2.185502	0.561658	-0.681549
O	-3.207195	0.510059	0.044636
O	-2.139827	0.3979	-1.918838

X=COO$^-$ (β)

Charge = -1 Multiplicity = 2

C	-1.564134	-0.757511	-0.253252
C	-0.200185	-0.173425	0.05072
H	-0.007042	-0.525606	1.199746
C	0.870478	-0.722702	-0.870189
H	0.722786	-1.799322	-0.970547
H	0.749842	-0.279741	-1.859072
C	-0.225484	1.340152	0.109418
F	-2.535537	-0.190035	0.467526
F	-1.895084	-0.611521	-1.542592
F	-1.582815	-2.066136	0.011237
F	-0.911346	1.803116	1.156714
F	-0.782005	1.867109	-0.990968
F	1.012857	1.830937	0.199412
O	0.501024	-0.943109	2.306377
H	1.414323	-0.95069	1.894976
O	3.146922	-0.215661	-1.307874
C	2.329168	-0.521852	-0.419302

O	2.615354	-0.732961	0.791318

X=-SO_3^- (α)

Charge =-1 Multiplicity = 2

C	1.848185	-0.956385	-0.004454
C	0.647129	-0.081804	-0.350032
H	0.484483	-0.171636	-1.424642
C	-0.577466	-0.553832	0.413056
H	-0.764662	-1.687297	0.099898
H	-0.454222	-0.563382	1.494149
C	0.984741	1.381991	-0.068887
F	2.832508	-0.825383	-0.895457
F	2.354032	-0.651046	1.197343
F	1.515427	-2.248054	0.022627
F	2.240943	1.67762	-0.42452
F	0.865107	1.686446	1.226489
F	0.184173	2.196624	-0.751886
O	-1.315401	-2.880052	-0.192992
H	-2.230346	-2.588276	-0.017248
S	-2.142101	0.227809	0.000943
O	-3.14342	-0.73435	0.476934
O	-2.170136	1.492179	0.734903
O	-2.134405	0.384715	-1.453433

X=-SO_3^- (β)

Charge =-1 Multiplicity = 2

C	-1.905222	-0.844932	-0.282396
C	-0.584892	-0.187667	0.098161
H	-0.497743	-0.437507	1.281629
C	0.577562	-0.813215	-0.642364
H	0.576837	-1.883822	-0.453958
H	0.487498	-0.647629	-1.717526
C	-0.688639	1.327266	0.015849
F	-2.847285	-0.647894	0.640965
F	-2.372325	-0.358469	-1.440043
F	-1.768547	-2.161949	-0.427822
F	-1.893404	1.762234	0.402031
F	-0.496884	1.765299	-1.232355
F	0.209572	1.918131	0.798763
S	2.237391	-0.267267	-0.19367
O	3.100642	-1.275969	-0.809125
O	2.418806	1.06956	-0.756638

O	2.291539	-0.286385	1.277737
O	-0.188065	-0.698909	2.513506
H	0.778788	-0.606036	2.375384

X=-PO_4^{2-} (α)

Charge =-2 Multiplicity = 2

C	-2.226797	0.921001	0.13337
C	-1.132712	0.081113	-0.500265
H	-1.194963	0.224542	-1.579162
C	0.234032	0.514926	0.019457
H	0.390456	1.610207	-0.324061
H	0.266384	0.534829	1.111828
C	-1.366338	-1.399513	-0.223282
F	-2.461109	0.564217	1.403843
F	-1.890473	2.214358	0.142682
F	-3.385482	0.823679	-0.522975
F	-2.667112	-1.721408	-0.260257
F	-0.911629	-1.761309	0.981375
F	-0.752522	-2.164217	-1.126263
O	1.120743	2.805231	-0.74938
H	1.975209	2.338829	-0.52484
O	1.218557	-0.291382	-0.530531
P	2.756059	-0.200271	0.156414
O	2.569268	-0.597089	1.606064
O	3.16146	1.26163	-0.026738
O	3.528456	-1.179313	-0.695827

X=-PO_4^{2-} (β)

Charge =-2 Multiplicity = 2

C	-2.137017	-1.028925	-0.180884
C	-0.986668	-0.117616	0.183408
H	-0.916514	-0.166815	1.393219
C	0.341848	-0.618241	-0.365796
H	0.311436	-1.706144	-0.442667
H	0.487309	-0.208876	-1.371023
C	-1.282066	1.334746	-0.13087
F	-3.32373	-0.513898	0.149753
F	-2.165602	-1.276354	-1.497213
F	-2.021189	-2.204793	0.4387
F	-2.1827	1.859401	0.704784
F	-1.770359	1.474306	-1.373229

F	-0.18287	2.081375	-0.051768
O	1.37208	-0.212574	0.505385
P	2.916015	-0.142064	-0.155494
O	3.127321	-1.501897	-0.801497
O	2.864967	1.005474	-1.151666
O	3.755077	0.126585	1.078572
O	-0.480697	-0.146194	2.617984
H	0.469019	-0.158452	2.388265

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(4-4) Formula: $(CF_3)_2$-CF_2-CH_2-X

X=-OH

Charge =0 Multiplicity = 2

C	-0.520983	-1.208252	-0.023412
C	0.078403	0.185343	-0.289923
C	-0.769347	1.266614	0.369376
H	-1.881553	0.984938	0.226761
H	-0.595533	1.289393	1.445188
C	1.544898	0.228422	0.182601
F	0.347839	-2.181526	-0.287813
F	-0.895816	-1.323168	1.248676
F	-1.58441	-1.391825	-0.795124
F	2.330815	-0.454995	-0.642733
F	1.645256	-0.307646	1.39925
F	2.003441	1.471917	0.240023
O	-0.523958	2.479198	-0.263639
H	-0.726287	3.194163	0.350029
O	-3.344604	0.791427	0.266541
H	-3.338586	0.017977	0.857383
F	0.096499	0.355662	-1.643882

X=-COO^-

Charge = -1 Multiplicity = 2

C	-1.539206	0.816452	0.236495
C	-0.240491	0.102296	-0.187512
C	0.924963	0.524482	0.677423
H	1.075631	1.683306	0.451337
H	0.678031	0.445939	1.734238
C	-0.445725	-1.427479	-0.179066
F	-2.468831	0.728707	-0.708914
F	-2.025103	0.278199	1.35392
F	-1.314456	2.107273	0.460476
F	-1.607926	-1.769879	-0.734738
F	-0.423578	-1.910101	1.057987
F	0.522254	-2.008017	-0.879825
O	1.562901	2.766541	-0.19753
H	2.247013	2.229471	-0.647022
F	-0.030486	0.439963	-1.49945
C	2.260889	-0.157339	0.331132

O	2.579396	-1.127957	1.045868
O	2.903937	0.323354	-0.630151

X=-SO_3^-

Charge =-1 Multiplicity = 2

C	1.86429	0.908303	-0.213528
C	0.639131	0.086895	0.25099
C	-0.603111	0.578164	-0.45621
H	-0.769518	1.704896	-0.079878
H	-0.467754	0.64304	-1.534379
C	0.912905	-1.420294	0.040536
F	2.884585	0.758599	0.621314
F	2.249989	0.523761	-1.427463
F	1.568027	2.203376	-0.258748
F	2.148916	-1.739314	0.425139
F	0.781816	-1.7554	-1.237603
F	0.068709	-2.13979	0.763681
O	-1.268225	2.873517	0.295649
H	-2.195597	2.648914	0.090131
F	0.551487	0.276162	1.601382
S	-2.187505	-0.212491	-0.109641
O	-3.146374	0.782915	-0.595596
O	-2.185617	-1.447779	-0.888997
O	-2.240795	-0.416397	1.333735

X=-PO_4^{2-}

Charge =-2 Multiplicity = 2

C	2.137176	-0.934019	0.346915
C	1.053738	-0.069948	-0.321553
C	-0.317787	-0.427919	0.215815
H	-0.520058	-1.51239	-0.172524
H	-0.312392	-0.497295	1.30643
C	1.376283	1.427462	-0.132117
F	3.254655	-0.944729	-0.369848
F	2.421	-0.465985	1.562298
F	1.725238	-2.192724	0.473954
F	2.687845	1.659285	-0.236548
F	0.983536	1.845394	1.067369
F	0.76868	2.15568	-1.057422
O	-1.163672	-2.66291	-0.73674
H	-2.039624	-2.173747	-0.724155

F	1.119008	-0.313576	-1.667098
O	-1.256869	0.453755	-0.277242
P	-2.868481	0.197569	0.183738
O	-3.532653	1.454879	-0.319171
O	-3.259074	-1.070053	-0.573904
O	-2.817333	0.018871	1.685241

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(4-5) Formula: $(CF_3)_3$-C-CH_2-OH

X=-OH

Charge =0 Multiplicity = 2

C	-0.511291	1.344833	0.271217
C	0.068316	-0.021859	-0.154595
C	-0.758864	-0.576519	-1.327196
H	-1.874444	-0.345182	-1.137677
H	-0.519131	-0.037406	-2.244335
C	1.533042	0.179257	-0.59985
F	0.379144	2.074341	0.940291
F	-0.892865	2.046311	-0.792116
F	-1.574605	1.186568	1.057183
F	2.35015	0.334394	0.441703
F	1.634585	1.26597	-1.364918
F	1.973829	-0.853413	-1.306691
O	-0.569657	-1.948194	-1.431711
H	-0.802984	-2.225758	-2.324804
O	-3.33053	-0.157515	-0.984273
H	-3.379477	-0.422481	-0.049228
C	0.035251	-0.977464	1.056741
F	0.372208	-0.340007	2.180598
F	-1.178875	-1.487199	1.233499
F	0.88963	-1.983962	0.90001

X=-COO^-

Charge = -1 Multiplicity = 2

C	1.430934	0.769249	-0.58156
C	0.206417	-0.04168	-0.07784
C	-1.051855	0.471028	-0.788275
H	-1.140881	1.625925	-0.581212
H	-0.915006	0.377693	-1.86094
C	0.425262	-1.525282	-0.449662
F	2.575097	0.106705	-0.407894
F	1.331264	1.048863	-1.877409
F	1.530343	1.925248	0.072255
F	1.3379	-2.110906	0.324847
F	0.836142	-1.627317	-1.713494
F	-0.702209	-2.219633	-0.332114
O	-1.211689	3.010952	-0.582094

H	-0.582018	3.174346	-1.30596
C	0.163523	0.079073	1.463919
F	1.402476	0.050524	1.974575
F	-0.391751	1.219595	1.848219
F	-0.498237	-0.931261	2.018275
C	-2.428516	-0.088379	-0.374234
O	-2.779487	0.059075	0.81226
O	-3.087063	-0.609825	-1.301582

X=-SO_3^-

Charge =-1 Multiplicity = 2

C	1.644863	0.914768	-0.704877
C	0.565243	-0.020413	-0.082271
C	-0.776726	0.419631	-0.673916
H	-0.87654	1.596847	-0.454761
H	-0.757584	0.352805	-1.758893
C	0.906007	-1.478115	-0.46065
F	2.874021	0.426679	-0.571849
F	1.433296	1.102233	-2.003142
F	1.604487	2.106913	-0.112669
F	1.987181	-1.907895	0.190095
F	1.148071	-1.573012	-1.766587
F	-0.092346	-2.296958	-0.165712
O	-1.232698	2.868059	-0.356895
H	-2.18915	2.677127	-0.400423
C	0.655204	0.123767	1.462672
F	1.919733	0.332424	1.844386
F	-0.063482	1.154335	1.88634
F	0.245869	-0.971275	2.089639
S	-2.38617	-0.245881	-0.158672
O	-3.287557	0.864676	-0.480534
O	-2.306888	-0.542925	1.264952
O	-2.607482	-1.416252	-1.003452

X=-PO_4^{2-}

Charge =-2 Multiplicity = 2

C	-1.856414	1.014177	0.658008
C	-0.903491	-0.038425	0.056545
C	0.532081	0.292011	0.50064
H	0.64753	1.452959	0.421088
H	0.667201	0.058595	1.55895

C	-1.311232	-1.434386	0.568617
F	-3.11969	0.592543	0.681294
F	-1.5068	1.310736	1.907
F	-1.816461	2.14153	-0.049968
F	-2.393019	-1.896284	-0.060904
F	-1.590003	-1.383042	1.871805
F	-0.338556	-2.321039	0.400342
O	1.240429	2.750155	0.233756
H	2.134518	2.31245	0.124836
C	-1.023489	-0.002204	-1.480307
F	-2.295915	0.148637	-1.861792
F	-0.331565	1.008857	-1.992137
F	-0.578518	-1.130718	-2.025065
O	1.444951	-0.332883	-0.317843
P	3.078214	-0.235259	0.12614
O	3.1232	-0.737196	1.552226
O	3.405461	1.249738	-0.012476
O	3.721903	-1.120207	-0.912311

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