

# Supporting Information

## **Thermodynamic and Optical Properties of $\text{HCOOH}(\text{H}_2\text{O})_n$ and $\text{HCOOH}(\text{NH}_3)(\text{H}_2\text{O})_{(n-1)}$ Cluster at Various Temperatures and Pressures: A Computational Study**

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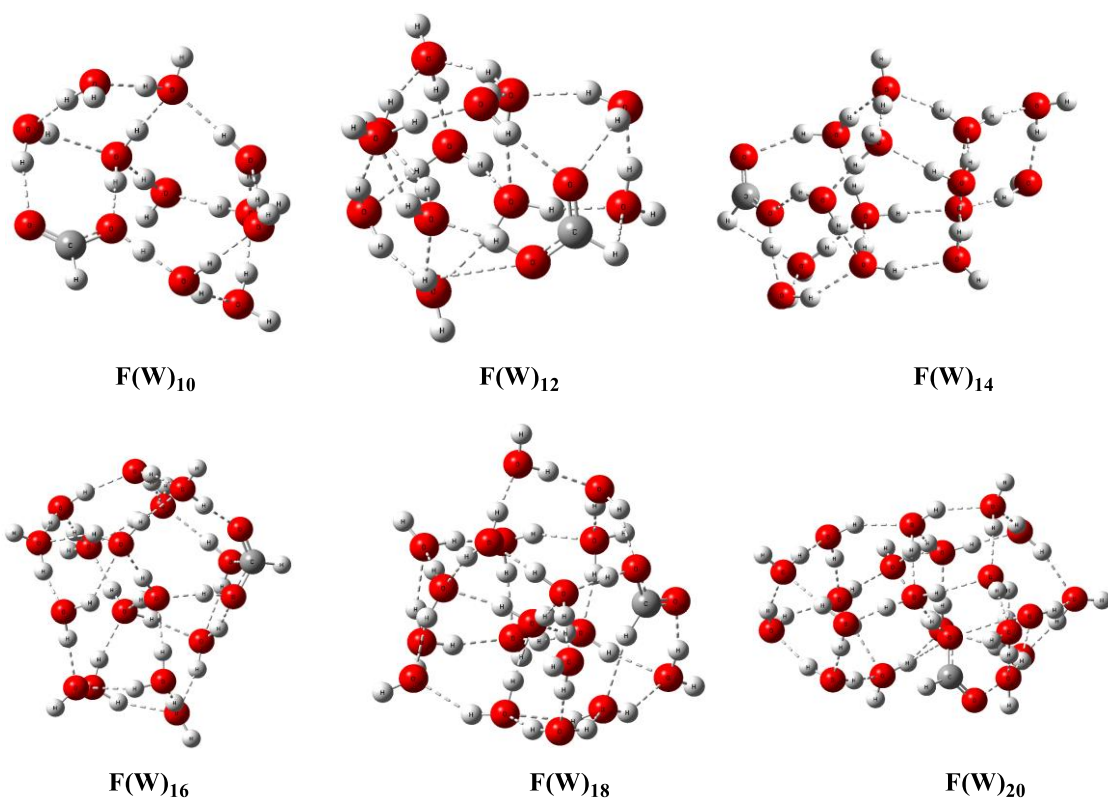


Figure S1. The identified lowest energy structures of  $F(W)_n$  ( $n = 10, 12, 14, 16, 18, 20$ ) clusters. Where  $F = \text{HCOOH}$  and  $W = \text{H}_2\text{O}$ .

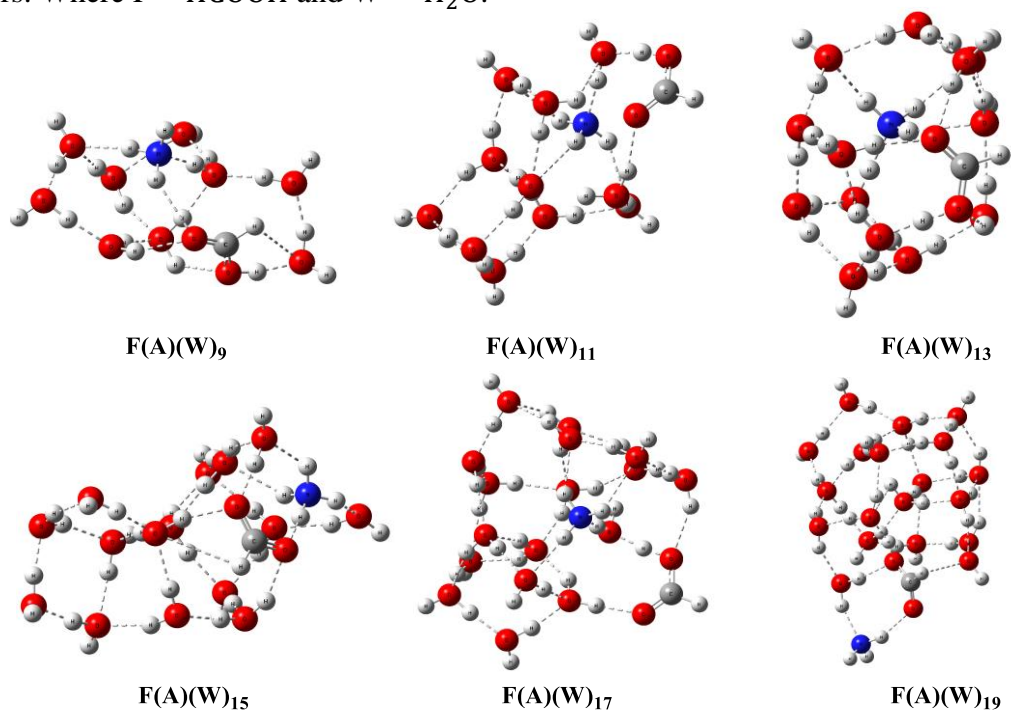


Figure S2. The identified lowest energy structures of  $F(A)(W)_{n-1}$  ( $n = 10, 12, 14, 16, 18, 20$ ) clusters. Where  $F = \text{HCOOH}$ ,  $A = \text{NH}_3$  and  $W = \text{H}_2\text{O}$ .

Table S1. The Cartesian coordinates of  $F(W)_n$ , and  $FA(W)_{n-1}$  ( $n = 1-8, 10, 12, 14, 16, 18, 20$ ) (where  $F = \text{HCOOH}$ ,  $A = \text{NH}_3$ , and  $W = \text{H}_2\text{O}$ ) clusters optimized at the M06-2X/6-31++G(d,p) level of theory.

$F(W)_1$			
Symbol	Coordinate		
	X	Y	Z
C	-1.19879900	-0.04667700	0.00747100
O	-0.64894200	-1.12686300	0.00402300
H	-2.28984200	0.07177800	0.01313100
O	-0.58949000	1.12736500	0.00614700
H	0.38750800	0.98203500	-0.00015500
O	1.87421700	0.01131000	-0.07885300
H	1.37542400	-0.81986700	-0.01692700
H	2.63342100	-0.04838700	0.50858800

$F(W)_2$			
Symbol	Coordinate		
	X	Y	Z
C	-1.63260000	-0.43095100	0.00674500
O	-0.74381100	-1.26211000	0.03907300
H	-2.69334700	-0.71505100	0.01662300
O	-1.47964600	0.86803300	-0.04271700
H	-0.50424400	1.13435400	-0.04876200
O	1.02624800	1.55581200	-0.06603100
H	1.58451200	0.74460900	-0.04160800
H	1.34454500	2.15381900	0.61720100
O	2.00746800	-0.92007400	0.06402100
H	2.49198300	-1.41080800	-0.60606900
H	1.09007500	-1.25450300	0.06737600

$F(W)_3$			
Symbol	Coordinate		
	X	Y	Z
C	2.12195800	-0.51666900	-0.08297500
O	1.17504300	-1.27040700	0.04767000
H	3.15021700	-0.89191100	-0.17814900
O	2.07748200	0.78736600	-0.12817800
H	1.13786700	1.15999500	-0.02129200
O	-2.51410300	0.67415200	-0.13753700
H	-3.01314000	0.78548100	-0.95225100
H	-2.29775900	-0.28357900	-0.05638100
O	-1.54570800	-1.81240700	0.04614800
H	-1.71820800	-2.44010100	0.75386000
H	-0.58208700	-1.65824700	0.03375900
O	-0.19921700	1.92773300	0.16559000
H	-0.27963300	2.48874100	0.94287100

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H	-1.07698300	1.48814100	0.02588200
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F(W)<sub>4</sub>

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Symbol	Coordinate		
	X	Y	Z
C	-2.61116400	0.29458500	-0.54256000
O	-1.88841700	1.25252300	-0.37192600
H	-3.58920700	0.37096600	-1.03638700
O	-2.35460600	-0.94524600	-0.18067900
H	-1.46707300	-1.02238700	0.27205200
O	2.79856300	0.97282800	-0.54513700
H	2.04226800	1.33089800	-0.01777500
H	3.60924200	1.33914400	-0.18082600
O	-0.01147600	-1.26441800	1.03741200
H	0.74780400	-1.45688800	0.41385600
H	0.00147700	-1.93695500	1.72651600
O	0.63774300	1.51735400	0.92390200
H	-0.16904800	1.71495200	0.42099200
H	0.44605000	0.64828300	1.31046700
O	2.02970600	-1.56109600	-0.56087400
H	2.44705300	-0.66354200	-0.61067000
H	1.90630200	-1.86753600	-1.46445100

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F(W)<sub>5</sub>

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Symbol	Coordination		
	X	Y	Z
C	-2.68512000	-0.83722600	0.47489900
O	-2.11856800	-0.03571300	1.19466900
O	-2.21248200	-1.35294300	-0.63193600
H	-3.69110100	-1.21503600	0.70325200
H	-1.28121500	-1.00486600	-0.82770800
O	0.13458600	-0.34395400	-1.06366100
H	0.33265400	0.11552600	-0.22136000
H	0.92130500	-0.90845300	-1.23055700
O	-0.07380700	2.44273700	-1.37075600
H	-0.08223400	1.53745400	-1.72150400
H	-0.62318300	2.98561600	-1.94265400
O	0.32421800	1.34436300	1.14689300
H	0.19190400	2.07681900	0.51998100
H	-0.56238800	1.02229100	1.38915600
O	2.67447500	-0.09959000	1.40614800
H	2.84578300	-0.41881200	2.29671900
H	1.90703500	0.50159600	1.45986000
O	2.53659400	-1.58910300	-0.89904200
H	2.74234500	-1.14279400	-0.05218000
H	3.28969000	-1.45236400	-1.48092600

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F(W) <sub>6</sub>			
Symbol	Coordinate		
	X	Y	Z
C	-0.59270700	-2.16554500	0.10889800
O	-1.71797800	-1.87900900	0.47303000
H	-0.18673500	-3.17826500	0.25498100
O	0.25579100	-1.36647000	-0.47797500
H	-0.07044400	-0.32621900	-0.60619700
O	3.76020100	0.72154900	0.76326400
H	3.57830500	-0.11679000	0.28695200
H	4.08603900	0.48232800	1.63579200
O	-0.26282600	0.97894800	-0.82031700
H	-1.17331500	1.35571500	-0.73663000
H	0.38202300	1.55635400	-0.34548800
O	-2.74050000	1.94652100	-0.58978300
H	-3.26226300	1.27934600	-0.08928100
H	-3.22862700	2.14180800	-1.39506400
O	-3.86078600	-0.12369900	0.70624600
H	-4.12087500	-0.10445600	1.63188800
H	-3.14246000	-0.77936300	0.63058000
O	3.03566600	-1.55057400	-0.56869200
H	2.06068600	-1.56884000	-0.60069300
H	3.34803800	-1.69774100	-1.46653500
O	1.64218500	2.38758900	0.44925300
H	1.95946200	3.20543600	0.05531500
H	2.43237700	1.82511000	0.61078500

M(W) <sub>7</sub>			
Symbol	Coordinate		
	X	Y	Z
C	-0.44035200	2.22330700	0.38653000
O	0.75864100	2.14351500	0.60028700
H	-1.10823400	2.77958800	1.05272900
O	-1.07041500	1.70446300	-0.63648700
H	-0.46362000	1.09200200	-1.20271800
O	-1.20773300	-2.09848600	-1.22869500
H	-1.56027100	-2.85049100	-1.71355100
H	-1.97388700	-1.55207000	-0.89573200
O	-1.45344300	0.12494800	1.98220400
H	-0.73506700	-0.52659600	1.77388700
H	-1.68677300	-0.00731700	2.90584400
O	2.94612400	-1.56279800	0.70912000
H	3.58389200	-1.58962200	1.42798900
H	3.05165800	-0.70668700	0.25343600
O	-2.96989900	-0.42860500	-0.21454500
H	-2.58615600	-0.25693200	0.67393700
H	-2.84644800	0.41474000	-0.67020000
O	0.29811500	0.07080500	-2.00519400
H	-0.09294500	-0.81422100	-1.85920900

H	1.23057800	0.05601600	-1.72721600
O	0.22216700	-1.76586400	1.18542600
H	1.19156700	-1.72959700	1.07478800
H	-0.15324400	-2.12828900	0.36654000
O	2.65991200	0.78269300	-0.70067900
H	3.30212400	1.36861000	-1.11317500
H	2.02117700	1.34565600	-0.19802100

F(W) <sub>8</sub>			
Symbol	Coordinate		
	X	Y	Z
C	-3.94169000	-0.80479000	0.61901400
O	-2.76563200	-1.08571400	0.74910500
H	-4.73973600	-1.35530000	1.13618900
O	-4.41822300	0.15803700	-0.12728100
H	-3.67135600	0.65571700	-0.60021800
O	1.72187100	2.36853400	1.28316900
H	1.56674500	3.09573600	1.89318400
H	0.86943300	2.13346400	0.85943200
O	2.43710100	1.39846900	-1.34837800
H	2.99037800	0.60487300	-1.24578700
H	2.66243000	1.97226300	-0.60146500
O	1.35314100	-2.43050600	-1.29211900
H	1.09861700	-2.21984300	-2.19557800
H	2.23169200	-2.02963700	-1.13927000
O	3.58654300	-1.02292500	-0.47696500
H	4.47502100	-1.37906000	-0.38026200
H	3.23870500	-0.79807800	0.43577500
O	2.42312700	-0.33432000	1.74996700
H	1.53730100	-0.73866400	1.69827700
H	2.27814700	0.62839000	1.77084500
O	-0.09648500	1.14140200	-0.33794900
H	-0.11289200	0.24593100	0.07941700
H	0.68814400	1.13826300	-0.92928200
O	0.00101600	-1.32296000	0.79628900
H	-0.93886500	-1.51562400	0.94544500
H	0.32405300	-1.88586100	0.06084800
O	-2.55664800	1.44799600	-1.36107900
H	-1.63443900	1.35499900	-1.01483200
H	-2.69973200	2.37707000	-1.56487900

F(W) <sub>10</sub>			
Symbol	Coordinate		
	X	Y	Z
C	1.52415200	2.41290100	-0.79571800
O	2.67735900	2.24298800	-1.13327900
H	1.08809500	3.42170100	-0.70712200
O	0.69395800	1.43717100	-0.50465800

H	-0.26235200	1.80445000	-0.20409900
O	1.01476000	-1.30206000	-1.09382100
H	0.88082600	-0.35705600	-0.88701400
H	1.01223500	-1.75778000	-0.22813300
O	-3.55756000	1.10042900	-1.03979500
H	-3.45073600	0.13781600	-0.90362600
H	-4.42885800	1.33848300	-0.70865800
O	3.72264600	-0.35628100	-0.77773600
H	3.01641100	-0.88439500	-1.18222300
H	3.49851400	0.56727200	-0.99901300
O	-1.47562100	2.33232400	0.19285700
H	-1.68001700	2.10899800	1.13329200
H	-2.23335800	1.97862000	-0.32681000
O	-1.10718700	-2.17727300	-2.46452400
H	-1.12747100	-1.84936400	-3.36846500
H	-0.25773700	-1.87838300	-2.05585500
O	-2.14700500	1.31361900	2.55533200
H	-1.97582400	1.51577100	3.47851400
H	-1.92339400	0.36295000	2.39598200
O	-2.92829200	-1.57924300	-0.67215100
H	-3.56594400	-2.29762500	-0.60598700
H	-2.29498700	-1.82110800	-1.40285800
O	-1.57400900	-1.17241400	1.81146000
H	-0.65547800	-1.49254700	1.77381800
H	-1.98912500	-1.36015200	0.95169200
O	1.06633800	-2.15520000	1.54999200
H	1.21921200	-3.05270800	1.86266700
H	1.88570300	-1.62532800	1.76619700
O	3.26690500	-0.78244300	1.80414100
H	3.34107800	0.03698300	2.30191600
H	3.53995000	-0.58692900	0.86755800

M(W) <sub>12</sub>			
Symbol	Cooperativity		
	X	Y	Z
C	2.97624500	0.14434800	1.16681800
O	2.96370000	0.77592600	0.12349300
H	3.83058000	-0.46436600	1.47977500
O	2.00032900	0.11411700	2.04095000
H	1.20484000	0.63359200	1.71875300
O	1.07201000	2.39275000	-1.28869200
H	1.79067500	2.07152400	-0.71942100
H	0.68781100	1.56844900	-1.65199500
O	2.85498300	-0.97139800	-2.15234000
H	3.23372500	-0.19035800	-1.72295700
H	1.93339100	-0.71960700	-2.35069800
O	-0.26599700	1.30773500	1.51075500
H	-0.78859400	0.95872900	0.75619200

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H	-0.35396600	2.27269100	1.40014400
O	-1.11858700	-0.80872700	2.96754700
H	-0.82574200	-1.09685400	3.83781300
H	-0.82805900	0.11286100	2.84114400
O	-2.53602900	-2.28887000	-0.78201000
H	-3.02362500	-1.88948600	-0.02885800
H	-1.61959700	-2.33917200	-0.45756800
O	-0.82571400	3.56495500	0.05219600
H	-0.88114000	4.52314800	-0.00316000
H	-0.06566100	3.25631700	-0.52008100
O	-2.26188800	1.20255800	-0.35590700
H	-2.41040900	0.82974300	-1.24598500
H	-2.11471000	2.16042500	-0.43431200
O	-2.46034400	-0.44182800	-2.57599600
H	-3.03556000	-0.54249100	-3.33979700
H	-2.58005900	-1.23863600	-1.96978900
O	2.50601500	-2.40310600	0.05918900
H	2.69912300	-1.99268000	-0.82398800
H	2.75617100	-3.33054300	0.00747500
O	-0.06926700	-1.59959400	0.42747100
H	-0.33282700	-1.46042900	1.35405800
H	0.83646800	-1.98137500	0.42637900
O	-3.47099400	-0.75391700	1.29456100
H	-3.22829200	0.09265500	0.88231500
H	-2.87566100	-0.86184400	2.05138600
O	0.20328000	-0.14624900	-1.94383100
H	0.03251500	-0.54648600	-1.06696000
H	-0.63084700	-0.24671700	-2.43985400

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$F(W)_{14}$

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Symbol	Coordinate		
	X	Y	Z
C	3.85250000	-0.09269500	-1.47827600
O	3.50793300	0.34079200	-2.55641800
H	4.62027200	-0.87273000	-1.37027000
O	3.33108200	0.33289900	-0.34337600
H	3.63811600	-0.21507400	0.47035200
O	0.71174300	0.33374000	-2.23222500
H	1.61252200	0.59416500	-2.49008600
H	0.15743200	1.12757200	-2.15676800
O	1.70653000	2.18776000	1.04000100
H	1.52996800	1.37352300	1.56288500
H	2.24885300	1.87247900	0.29991900
O	-0.45291700	3.44652900	0.55555000
H	0.43318400	2.98385000	0.73681900
H	-0.35288500	4.37151000	0.80226300
O	-4.12958200	-2.97778500	-0.47234800
H	-3.87669200	-3.72856500	-1.01761700

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H	-3.31143700	-2.64190000	-0.04837600
O	-3.00479900	0.65992600	-0.63282000
H	-3.83283100	0.32904500	-1.04780700
H	-2.49911900	1.19162000	-1.27277400
O	-1.95144200	-1.60759200	0.47623700
H	-2.24646300	-0.76637900	0.05731100
H	-1.84060200	-1.39919500	1.42364900
O	-1.17457600	2.42037000	-1.82751600
H	-1.34617600	3.05276600	-2.53243700
H	-0.93666000	2.93096000	-1.01765500
O	0.72760900	-1.44707000	-0.27286300
H	0.73278800	-0.76685200	-0.99965600
H	-0.20512700	-1.70878100	-0.14746500
O	1.25159600	-0.28121000	2.12012100
H	0.42804100	-0.35377800	2.63672900
H	1.05407000	-0.70924600	1.25136400
O	-1.41841800	-0.39316000	2.96365000
H	-1.76715200	0.48186300	2.62344900
H	-1.81979500	-0.55242900	3.82345300
O	-5.16409500	-0.68612800	-1.52033700
H	-6.05665700	-0.52263400	-1.20226100
H	-4.90580800	-1.58059300	-1.20673500
O	3.85430500	-1.09365100	1.68217700
H	3.69947900	-1.97017200	1.28112400
H	3.06204000	-0.89945000	2.21739300
O	-2.34050000	1.76416600	1.82227500
H	-1.69357700	2.43134800	1.52874300
H	-2.77763400	1.45875900	1.00423200
O	3.04022400	-2.84084400	-0.23055400
H	3.05084600	-3.73740700	-0.57632800
H	2.12847500	-2.48804800	-0.33622500

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$F(W)_{16}$

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Symbol	Coordinate		
	X	Y	Z
C	-1.40748400	-2.65330800	-1.88526400
O	-2.27668800	-1.83426300	-2.11856500
H	-1.60203800	-3.72925100	-1.87809500
O	-0.14353900	-2.36961700	-1.65449900
H	0.01697700	-1.37210700	-1.52953300
O	-1.33431500	0.52262600	3.20362300
H	-1.22246800	0.70611500	4.14156100
H	-1.56576900	1.39963700	2.73146300
O	-0.63887500	2.22825300	-1.99652900
H	-1.48074800	1.88482700	-2.34943700
H	-0.84977400	2.89415500	-1.31868600
O	3.43772200	0.07222000	1.79395700
H	3.71830800	-0.81862300	1.52046900
H	2.46303200	0.01613400	1.86652100

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O	1.89043700	3.21484300	-1.02208500
H	1.49972800	2.75062000	-1.77466600
H	2.64339000	2.68175000	-0.69469500
O	1.06678100	-2.96407500	0.89100100
H	0.67403500	-2.99714900	0.00254400
H	2.03456900	-2.96201800	0.76277900
O	-2.90836000	0.75062800	-2.53336100
H	-2.61327700	-0.18333500	-2.44279800
H	-3.57605000	0.76657000	-3.22638400
O	4.02466400	1.70407900	-0.13498200
H	3.83851400	1.13922000	0.67533500
H	4.83588000	2.19617400	0.02476200
O	-3.11528000	-1.11991800	1.96549200
H	-3.90408300	-1.34117000	2.47120800
H	-2.53012000	-0.59362200	2.55447100
O	-0.32215700	3.98082700	0.17410200
H	-0.39924600	4.93997300	0.17605100
H	0.60291200	3.75934400	-0.10850100
O	-1.73526000	-3.29760300	0.70676200
H	-2.24213500	-2.58944700	1.13724500
H	-0.98496400	-3.48617400	1.28392300
O	0.71634200	-0.38413900	1.60666600
H	0.02612900	-0.11524000	2.24659400
H	0.71506700	-1.36447000	1.51347400
O	0.54476200	0.01924200	-1.05860000
H	0.09610900	0.84123600	-1.37885700
H	0.52978400	0.02676500	-0.07131200
O	3.25042700	-0.58868500	-1.55310800
H	2.30194000	-0.36213700	-1.50990500
H	3.71319400	0.22655700	-1.29190600
O	-3.58903600	1.08886700	0.22446300
H	-3.49526800	0.20120300	0.60959800
H	-3.45557400	1.00633100	-0.73379500
O	3.73059900	-2.34671900	0.33885100
H	4.44953500	-2.95455500	0.14088000
H	3.59631400	-1.75859100	-0.45767600
O	-2.02352800	2.55866500	1.87115300
H	-2.63508600	2.16592200	1.20649800
H	-1.35149700	3.06335000	1.37772400

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$F(W)_{18}$

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Symbol	Coordinate		
	X	Y	Z
C	2.39713100	-1.48569600	1.11752800
O	2.28429000	-1.95602000	2.24012400
H	2.46694900	-0.39550700	0.95339700
O	2.43762600	-2.22584500	0.04082800
H	2.42702800	-1.61834000	-0.80230900

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O	-1.67767700	0.76159500	-2.22883100
H	-2.55830400	0.40096300	-2.00162700
H	-1.74530000	1.73392000	-2.18222800
O	0.25639400	-0.94254400	-3.46867100
H	-0.45334800	-0.30996100	-3.26467900
H	-0.13450600	-1.83768400	-3.35803400
O	4.11894400	1.12806000	-2.28064200
H	4.46451500	1.47736100	-3.10624100
H	3.89166100	1.89092500	-1.69047300
O	-1.85842700	3.44665100	-1.36733400
H	-2.20464100	4.20748900	-1.84429200
H	-2.57328100	3.13823800	-0.74769600
O	-0.41859500	0.03915500	2.24873100
H	-0.07670900	0.26465100	1.34789000
H	0.30294800	0.16864200	2.89262900
O	0.20486300	0.49608300	-0.31248300
H	-0.54375500	0.45647700	-0.95251100
H	0.99229100	0.17188800	-0.80199500
O	-3.71569300	2.33429200	0.13714900
H	-3.43505800	1.98798500	1.00286300
H	-4.06077900	1.56909900	-0.35649800
O	-0.81344600	-3.35850300	-2.85598300
H	-0.75560800	-4.16394300	-3.37713400
H	-0.51742900	-3.58092900	-1.94206900
O	0.63071000	3.17983100	0.02261400
H	0.46453000	2.22909800	-0.15298200
H	-0.14130500	3.62234600	-0.36484800
O	3.38610600	2.97637100	-0.51805500
H	3.43309900	2.55166900	0.35368900
H	2.45766200	3.26929300	-0.56475000
O	-2.91927300	0.99621200	2.50686000
H	-3.13743500	1.33988300	3.37872300
H	-1.96240800	0.75419000	2.50729700
O	0.05091400	-3.82350600	-0.34652700
H	-0.46306000	-3.36603300	0.34189900
H	0.96885200	-3.55311300	-0.19576600
O	-1.25400400	-2.51720500	1.80758200
H	-0.83923100	-1.65388200	2.03516300
H	-1.09057700	-3.11026400	2.54898700
O	1.83084800	0.05093400	3.91872700
H	2.12609500	-0.76582300	3.44254000
H	1.97251700	-0.08062500	4.86070000
O	-3.71350700	-1.31739100	1.08075400
H	-2.96356400	-1.91377200	1.25230200
H	-3.61960300	-0.59125200	1.72112900
O	2.20164900	-0.60209500	-1.81972300
H	1.52734700	-0.76428700	-2.55377000
H	2.93728100	-0.00834500	-2.12413900
O	-4.10429700	-0.11372500	-1.21356800
H	-3.95415400	-0.68344700	-0.40876300

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H	-4.82649000	-0.50417300	-1.71527700
O	2.24940800	1.77384200	1.76264500
H	2.25757700	1.51796700	2.69713200
H	1.56875100	2.45393700	1.63299200

F(W) <sub>20</sub>			
Symbol	Coordination		
C	-0.72882500	0.41089800	-2.23933200
O	-1.43925200	-0.11992300	-3.06946100
H	-0.12249300	1.30153400	-2.46471600
O	-0.63490500	-0.03026200	-0.99917600
H	-0.17335400	0.66731900	-0.37787400
O	0.10044100	-2.85315800	-1.17053700
H	0.00654800	-2.40851600	-0.29428700
H	0.62582900	-3.64137600	-0.96163900
O	-2.93331900	2.34353100	-1.92644300
H	-2.93788000	2.12728000	-2.86501400
H	-3.23012900	1.54126700	-1.45645000
O	-2.07694800	0.60147000	3.49692600
H	-2.49102600	0.79583000	4.34381400
H	-2.23262800	1.37345500	2.90929100
O	3.33886700	-0.05495700	2.19404100
H	3.21592800	-0.61579000	1.40251100
H	2.47720700	-0.01952700	2.64235000
O	-2.52917500	-2.00595500	2.31319000
H	-3.23221800	-2.11927300	1.65073400
H	-2.57433300	-1.09963200	2.66054000
O	-3.26026800	0.24177600	-0.16259900
H	-3.93084000	-0.45148900	-0.02367300
H	-2.42737200	-0.22861800	-0.35022700
O	-2.31255200	2.29825500	1.40462200
H	-2.67117600	3.15459200	1.08941400
H	-2.77210000	1.61026200	0.87989900
O	4.40860600	2.15029100	1.30225800
H	4.99929200	2.59534800	1.91699200
H	4.01049400	1.36117300	1.76689400
O	-3.27142400	4.37162800	-0.09425600
H	-2.85580900	5.22387700	-0.25377700
H	-3.19193700	3.84987600	-0.91614100
O	5.04201300	0.45507900	-0.90274900
H	4.75985400	-0.39605700	-0.53427100
H	5.06105700	1.07943600	-0.15727200
O	0.60329700	0.08559300	2.70671400
H	0.51019600	0.73830400	1.97649600
H	-0.18127900	0.21328000	3.26700400
O	3.21084700	-1.62734400	-0.10875800
H	2.74187700	-1.40577700	-0.93324500
H	2.94192700	-2.53530300	0.12099300

O	0.01341700	-2.28269300	1.47442400
H	-0.92450900	-2.33401800	1.77847000
H	0.34774800	-1.45869600	1.89092000
O	2.88667200	1.43468700	-2.32385500
H	2.33068400	0.64814300	-2.43275900
H	3.73766000	1.08972100	-1.97697500
O	2.22683900	2.99421100	-0.22672600
H	3.00282800	2.88703400	0.35679400
H	2.46205700	2.53175500	-1.06828000
O	1.70807100	-1.15918400	-2.51347300
H	1.00761300	-1.75168800	-2.14999900
H	1.98898700	-1.53369400	-3.35535800
O	0.24482300	1.69312700	0.56096200
H	1.03895400	2.29575500	0.27834300
H	-0.55743500	2.20192700	0.79607600
O	1.89177200	-4.01438700	0.67913900
H	1.22958800	-3.54691000	1.23562200
H	2.24777800	-4.74915000	1.18749500
O	-2.56710300	-2.46543500	-1.88947800
H	-2.37862500	-1.66681700	-2.41515700
H	-1.68412600	-2.81484700	-1.66952100
O	-4.28049200	-2.27007100	0.08481400
H	-3.68952900	-2.45920200	-0.69577200
H	-5.07419200	-2.80639900	0.00113000

FA

Symbol	Coordinate		
	X	Y	Z
N	1.93594400	0.08804000	-0.00004700
H	2.52978700	0.02355400	0.82065400
H	2.52904800	0.02507300	-0.82141900
H	1.48266500	1.00110200	0.00090900
C	-1.25161600	-0.06017200	-0.00007500
O	-0.88613900	1.09647100	0.00007800
O	-0.46062700	-1.11607500	0.00005800
H	-2.31242400	-0.35008200	-0.00037200
H	0.50313800	-0.79807000	-0.00007700

E(A)(W)<sub>1</sub>

Symbol	Coordination		
	X	Y	Z
C	1.66852200	-0.51586700	-0.01201500
O	0.73644200	-1.29572200	-0.00345300
O	1.58449300	0.79257100	0.00648200
H	2.71495800	-0.85257800	-0.03761300
H	0.61802600	1.10031000	0.02882400
O	-0.87741000	1.57170500	0.07545100
H	-1.49855800	0.78578900	0.00554500
H	-1.17693300	2.25548300	-0.53076700
N	-2.20453100	-0.76732300	-0.00710500

H	-2.74225100	-1.08341300	-0.80759000
H	-1.31868200	-1.27582500	0.00571200
H	-2.72418200	-1.01173000	0.82987200

F(A)(W)<sub>2</sub>

Symbol	Coordinate		
	X	Y	Z
C	-2.07130700	0.61724200	-0.14376500
O	-2.42394800	-0.41683700	-0.66426800
O	-1.01141900	0.75229200	0.63821400
H	-2.60838300	1.56837800	-0.27342600
H	-0.57074800	-0.17203400	0.71848500
O	2.38523400	-1.01015500	-0.42961100
H	2.34099600	-0.02729000	-0.29509000
H	3.22807100	-1.32137800	-0.08778500
N	1.87537800	1.68407000	-0.05429700
H	1.96793500	2.21843600	-0.91306900
H	2.36854900	2.19332700	0.67275100
H	0.88668800	1.67412100	0.19609600
O	-0.01992500	-1.58723200	0.59162500
H	0.88053200	-1.56445600	0.19049900
H	-0.63298300	-1.96558800	-0.05347500

F(A)(W)<sub>3</sub>

Symbol	Coordinate		
	X	Y	Z
C	-0.25682100	-0.96547000	0.94204100
O	-1.37681000	-0.75175300	1.34971300
O	-0.00601100	-1.40566500	-0.27865300
H	0.64128500	-0.80019800	1.55960700
H	0.98654500	-1.39370500	-0.43888700
O	-2.42510900	-0.12038500	-1.26866700
H	-1.74316700	-0.69958100	-1.63042300
H	-2.53243500	-0.45607300	-0.36510800
N	-0.79307700	2.02116200	0.10394100
H	-1.31349700	1.43768000	-0.55926900
H	-1.18283400	1.80602900	1.01923900
H	-1.02092800	2.98955400	-0.10312900
O	1.85865200	1.51297600	0.01384500
H	0.87173000	1.72865500	0.03295100
H	2.30359000	2.11333300	0.61870400
O	2.51999900	-0.97784100	-0.44042500
H	2.43116800	0.00397500	-0.31948500
H	3.08523700	-1.14365100	-1.20053200

F(A)(W)<sub>4</sub>

Symbol	Coordinate		
	X	Y	Z

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C	-0.75450200	-1.01993900	-1.00839800
O	-1.89234200	-0.71179200	-1.28518700
O	-0.44159800	-1.76052600	0.03699700
H	0.11036500	-0.68834400	-1.60884600
H	0.55732000	-1.86992200	0.09710600
O	2.97037800	0.60878000	0.50377500
H	3.19013300	0.89951200	1.39377900
H	2.30050500	1.24528900	0.14690400
N	-2.33460200	-0.06290800	1.62588900
H	-1.58172700	-0.65427600	1.96598300
H	-2.79631000	-0.59910600	0.89266300
H	-2.99225500	0.08660400	2.38380200
O	2.12058500	-1.84223800	0.17266700
H	2.70625800	-2.34857500	-0.39694000
H	2.51116600	-0.93524700	0.30501000
O	1.10437500	2.20326600	-0.48518700
H	1.26193800	3.08759300	-0.82640100
H	0.12903300	2.12348600	-0.29390600
O	-1.47604200	1.92562500	-0.08907700
H	-1.75187600	1.32066900	0.65070300
H	-1.85817500	1.50739900	-0.87259500

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$F(A)(W)_5$

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Symbol	Coordinate		
	X	Y	Z
C	1.64067600	-1.83242700	1.03115500
O	1.49165400	-0.87881800	1.77777500
O	1.75383300	-1.78201000	-0.26864100
H	1.68419300	-2.86169900	1.41785700
O	-3.43655000	-0.73388300	-0.92633500
H	-3.97897200	-0.38631300	-1.64023400
H	-2.52467900	-0.83034300	-1.27691900
O	-0.26814800	0.94321700	0.65826300
H	-1.16495700	0.91944900	1.06056800
H	0.33460700	0.42035600	1.22218100
O	-0.77015100	-0.70941600	-1.49458600
H	-0.54792000	-0.09840100	-0.75644000
H	-0.23616100	-1.50019200	-1.34275200
O	1.36741500	2.98144100	-0.13842200
H	0.63534000	2.46932200	0.25618000
H	1.64396100	3.63226000	0.51226600
O	-2.88472000	0.68610100	1.33245900
H	-3.25479400	0.28636200	2.12447500
H	-3.22740300	0.18047400	0.56342000
N	2.07984900	0.45886300	-1.45189500
H	2.08801600	1.32952400	-0.91031000
H	1.29289100	0.52565500	-2.09676500
H	2.93057900	0.43165100	-2.00767400
H	1.89562600	-0.78863400	-0.67361600

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F(A)(W)<sub>6</sub>

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Symbol	Coordinate		
	X	Y	Z
C	-3.11783400	-0.08551600	0.69313800
O	-2.33216200	0.85193600	0.80031500
H	-4.01536900	-0.14554000	1.32552200
O	-3.01609100	-1.08108300	-0.12727600
H	-2.16243800	-1.00932600	-0.74571800
O	1.77141800	-1.39044600	1.66651800
H	1.79862500	-1.81956700	2.52644500
H	1.19273400	-0.57914000	1.75542200
O	0.36285500	0.80409900	1.74942100
H	0.80828900	1.47003200	1.19256500
H	-0.57156200	0.79293300	1.48161900
O	-1.04061400	-0.88517600	-1.62206600
H	-0.23571500	-1.37518200	-1.36314700
H	-0.80852700	0.07257900	-1.69248800
O	1.73555500	2.25360100	-0.18408200
H	2.36493800	1.48680200	-0.38140800
H	2.24671200	3.06663800	-0.13296700
O	-0.72443800	1.77094700	-1.43878500
H	-1.33467700	1.80772500	-0.68613600
H	0.13840300	2.08472600	-1.11423800
O	1.24658000	-2.25157500	-0.83102200
H	1.39814900	-2.13538900	0.13375800
H	1.24558700	-3.19496700	-1.01868300
N	3.21386800	0.04365500	-0.55043200
H	2.71333400	-0.60551000	-1.15692600
H	4.16501500	0.12112600	-0.89704100
H	3.24160500	-0.40885900	0.36343500

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F(A)(W)<sub>7</sub>

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Symbol	Coordinate		
	X	Y	Z
C	0.86073400	0.72790300	-1.21129300
O	-0.17861100	0.69916700	-1.85406500
O	1.32950900	1.82902700	-0.68128400
H	1.46416400	-0.17932000	-1.04369200
H	2.17618000	1.61912400	-0.14400100
O	-0.23456900	-0.44885200	1.30448300
H	-0.55418800	-1.00460700	0.57170300
H	-0.98693600	0.10477100	1.57242100
O	2.39456200	-1.14064400	1.53569400
H	2.26990600	-1.79114900	0.82000800
H	1.47958100	-0.88345700	1.76547100

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O	-2.57944800	1.13206200	1.41969400
H	-2.22842800	1.79614500	0.77456600
H	-3.01056700	1.62440800	2.12466900
O	1.54144100	-2.59362300	-0.70463700
H	1.82991600	-3.42379400	-1.09410300
H	0.57149000	-2.53561800	-0.83182000
O	3.30988800	1.10247800	0.68993400
H	3.06732300	0.19337100	1.05846400
H	4.22798500	1.09948400	0.40562100
O	-1.43495700	2.74180700	-0.39297400
H	-0.54833300	3.00071700	-0.10688200
H	-1.24575100	2.15178800	-1.14483500
O	-1.04756000	-1.84662400	-1.05138500
H	-1.98059300	-1.84541500	-0.70584300
H	-0.94913400	-1.06239500	-1.61848500
N	-3.46798100	-1.52875300	0.21039000
H	-3.36825800	-0.59560700	0.61619600
H	-3.57545700	-2.18498100	0.97830200
H	-4.32948300	-1.54800100	-0.32642100

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F(A)(W)<sub>9</sub>

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Symbol	Coordinate		
	X	Y	Z
C	1.86718900	-1.72354300	0.36191400
O	0.84201400	-2.26275100	0.71994400
H	2.58909800	-1.30103700	1.07987000
O	2.20660600	-1.58792900	-0.90642300
H	3.08761500	-1.10311200	-0.96989600
N	-0.97553500	-0.01910900	1.89743800
H	-1.88925100	0.27486700	1.54691300
H	-1.00050900	0.03483800	2.91109800
H	-0.84126900	-0.99676600	1.64524200
O	-0.31010600	3.54864600	-0.10747300
H	-1.02866300	3.09295600	-0.61383400
H	-0.00706800	4.28637700	-0.64382800
O	-4.08906700	-1.82516800	0.21381800
H	-3.17560300	-2.05538200	-0.08768500
H	-4.69822200	-2.23222800	-0.40887200
O	-3.65155000	0.77198400	0.56331200
H	-4.36256000	1.26500800	0.98314500
H	-3.97136900	-0.15309800	0.42243300
O	3.44127200	1.04169200	1.27788000
H	2.47649300	1.18960700	1.05558200
H	3.74696600	1.80280100	1.77913700
O	0.94223100	1.23598800	0.54825200
H	0.62871400	2.15069200	0.35820500
H	0.23699800	0.81539900	1.15186700
O	-0.11313400	0.00058900	-1.66191000
H	0.55962800	-0.54240000	-2.09280600

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H	0.35387900	0.42856300	-0.90722100
O	4.37985000	-0.20918000	-0.83538900
H	5.25260300	-0.60248400	-0.74287200
H	4.21148000	0.37237300	-0.05106300
O	-2.07331400	2.01823200	-1.39801200
H	-2.69176500	1.58445000	-0.78060700
H	-1.53119000	1.31351600	-1.78740700
O	-1.60572900	-2.14023800	-0.66638800
H	-1.22506800	-1.32880100	-1.05492300
H	-0.84788900	-2.55604500	-0.22692300

F(A)(W) <sub>11</sub>			
Symbol	Coordinate		
	X	Y	Z
C	4.34506100	0.88341700	-0.86236000
O	3.15202400	0.74434500	-1.10466800
H	4.94839900	1.65623000	-1.35778800
O	5.02995600	0.16790000	-0.02335600
H	4.39962700	-0.50067900	0.45477100
N	1.05524300	-0.05126900	1.51998400
H	0.42286100	-0.67516900	2.01589300
H	0.67368600	0.07347700	0.58271400
H	1.02252700	0.86560500	1.96355600
O	-0.85802200	-0.03029100	-1.59170300
H	-1.68482600	0.08715700	-2.10206200
H	-1.16757100	-0.45650500	-0.76476100
O	-4.30627100	1.17572900	0.26326500
H	-4.96174100	1.82393000	0.53759800
H	-3.49416800	1.29928400	0.84439100
O	0.70219500	2.15679100	-0.99917400
H	0.09076000	1.46450100	-1.32434300
H	1.60135500	1.82964200	-1.16354400
O	-1.67606800	-1.34922200	0.71908100
H	-1.03844200	-2.09091200	0.80992200
H	-2.56840100	-1.69337300	0.53126100
O	0.03832900	2.77741900	1.46626000
H	0.03221300	3.72210100	1.64516900
H	0.32223300	2.65049100	0.52098700
O	-4.36013300	-1.52482200	-0.00164900
H	-5.07675300	-2.07069100	0.33534500
H	-4.55347900	-0.59268000	0.23943100
O	-3.51988500	0.11341800	-2.26747100
H	-3.86536600	-0.73818800	-1.96468700
H	-3.82087800	0.73834000	-1.58653300
O	-2.20389400	1.18624000	1.76894400
H	-1.85691600	0.29239800	1.59810800
H	-1.45382800	1.81089000	1.68437600
O	3.32371000	-1.30795400	1.04177500
H	3.38091700	-2.12809400	1.53928900

H	2.46306400	-0.81487800	1.29898600
O	1.43523800	-1.59094100	-1.29170500
H	2.16695200	-0.97188700	-1.13029400
H	0.72282900	-1.08683800	-1.72272500
O	0.52985900	-2.90726100	0.81453200
H	0.95531200	-2.47025800	0.02739000
H	0.58626400	-3.85632000	0.66877500

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F(A)(W)<sub>13</sub>

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Symbol	Coordinate		
	X	Y	Z
C	0.12732100	2.89977700	-0.68864000
O	-0.26914900	2.84638000	0.48026300
H	-0.57210800	3.15398800	-1.49882600
O	1.32688100	2.68022700	-1.09501100
H	2.02280200	2.32079200	-0.32463300
N	-1.16904900	-2.17229300	-0.41329200
H	-1.50693300	-2.28844800	0.54322600
H	-0.98507600	-1.17545500	-0.53221900
H	-1.95741800	-2.37039900	-1.02845600
O	2.50513100	-1.47112100	-2.09555500
H	2.01166700	-2.24987800	-1.76405300
H	1.85332100	-0.84985200	-2.48713800
O	-3.85095900	-0.33830300	0.77438700
H	-3.28102000	-0.79467400	1.42616800
H	-3.55093200	0.58334200	0.73666800
O	0.32665900	-0.89783600	2.88052800
H	1.03396300	-1.39330600	2.40635300
H	0.57044600	0.03993400	2.85647700
O	3.83415700	-0.49152300	-0.18855500
H	3.32717300	-0.86868100	-0.99912300
H	4.77682200	-0.57774200	-0.36352000
O	1.11270300	-3.42195500	-0.76690200
H	0.17483700	-3.01122600	-0.66219800
H	1.02097300	-4.35143300	-0.99631000
O	-1.79942900	0.61047900	-1.87509800
H	-2.46527200	-0.07018600	-2.08978400
H	-2.26778900	1.23630200	-1.29960100
O	1.10740300	1.86687000	2.64392600
H	1.13091000	2.42026500	3.43109900
H	0.53484900	2.30677700	1.98202600
O	-3.76612300	-1.33593900	-1.69241800
H	-3.91260800	-1.03323500	-0.75946500
H	-4.62662700	-1.47132500	-2.09866700
O	0.79075000	0.47845600	-2.99021600
H	1.18280800	1.30889000	-2.69099500
H	-0.13168300	0.50255600	-2.67452300
O	-2.11862000	-1.69286400	2.45298400
H	-2.41830800	-2.17583800	3.22839100

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H	-1.19741200	-1.36075500	2.65348300
O	2.90708800	1.82879100	0.55041300
H	2.51434200	1.73591800	1.43816600
H	3.30053800	0.94975800	0.27409900
O	2.25682200	-2.21538700	1.48954600
H	1.90394600	-2.78164100	0.77797500
H	2.93340600	-1.66143100	1.06816500
O	-2.91533400	2.31013200	0.15935400
H	-2.05025400	2.63594300	0.48220700
H	-3.53376800	3.04719100	0.16872100

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F(A)(W)<sub>15</sub>

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Symbol	Coordinate		
	X	Y	Z
C	0.61515800	1.84645300	1.76561700
O	0.36273900	2.43917300	0.68341900
H	-0.23507700	1.70562900	2.46091600
O	1.72401200	1.38226700	2.13090500
H	1.17775200	-0.33701100	2.81701700
N	3.64703000	1.25274500	0.29064100
H	3.63198900	2.13338000	-0.23234400
H	3.36934200	0.49500000	-0.35001000
H	4.57601900	1.01753200	0.66063600
O	-4.82280200	0.09532300	-1.87104200
H	-3.90346400	-0.21755000	-1.92013000
H	-4.77040200	1.04992300	-1.67059100
O	5.89275100	-0.38323900	0.65917600
H	5.29521600	-1.06301400	0.29125900
H	6.53670700	-0.82260000	1.22051600
O	0.66925400	-1.16663100	2.78103300
H	-0.27834400	-0.90644300	2.69344400
H	1.14726400	-2.04185600	1.63152100
O	-2.20863800	1.50859900	0.31447900
H	-1.34880000	1.97800300	0.31214500
H	-2.12134000	0.73717100	-0.28719300
O	-2.25288900	-0.84455900	-1.11488100
H	-2.58035700	-1.47559100	-0.44422900
H	-1.37472200	-1.16352700	-1.39738900
O	2.01177200	0.62089200	-2.03512800
H	1.21937900	0.18361800	-1.67762400
H	1.89817100	1.58651700	-1.97457200
O	-4.34275800	2.67066900	-0.92029200
H	-4.91005300	3.23445300	-0.38783200
H	-3.57726700	2.40964400	-0.36493800
O	0.39289500	-1.58843900	-1.47478100
H	0.93850700	-1.96102500	-2.18507800
H	0.69679900	-2.01225700	-0.64367400
O	-1.92412100	-0.41528300	2.40344300
H	-2.50245100	-1.12965100	2.08453000

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H	-2.09265200	0.33388000	1.80265200
O	-5.79843500	-1.28171800	0.15378800
H	-5.52968700	-0.73937600	-0.63989000
H	-6.33334900	-0.71780400	0.71992700
O	-3.51317200	-2.25378800	0.94431800
H	-3.57013700	-3.20900300	1.04313000
H	-4.43313000	-1.92442700	0.73294500
O	2.12305100	3.20501500	-1.07189300
H	1.95876700	4.09470800	-1.39761500
H	1.43908300	3.00480400	-0.36682200
O	2.73275800	-1.69836500	-3.10732200
H	2.61686300	-0.72708000	-3.04246800
H	3.08441200	-1.90705600	-3.97765100
O	3.72074200	-1.61158100	-0.44403400
H	3.54526300	-1.81743800	-1.37774600
H	3.00122500	-2.02548200	0.07319300
O	1.46794800	-2.60479700	0.84228500
H	2.91067900	1.32432000	1.06405700
H	1.41677400	-3.52662800	1.11392300

F(A)(W) <sub>17</sub>			
Symbol	Coordinate		
	X	Y	Z
C	-2.72525300	3.83244500	-0.68927800
O	-1.60511400	4.20707900	-0.37490300
H	-3.55032100	4.55072400	-0.80151300
O	-3.08703300	2.60550800	-0.92330100
H	-2.28161700	1.88787600	-0.80931100
N	-1.43396000	0.42971500	1.97109600
H	-2.39571500	0.56374500	2.27725800
H	-0.81300000	0.99472100	2.54609900
H	-1.22658100	-0.55739000	2.12379100
O	-1.34829200	0.90139800	-0.63163500
H	-1.66725200	0.09777200	-1.10114200
H	-1.34256300	0.69514200	0.37495700
O	-2.54635600	-1.12928200	-2.05608900
H	-2.47343700	-2.03744000	-1.72305600
H	-3.42469200	-0.78227700	-1.78812400
O	2.00568200	-3.08294700	0.95142000
H	2.02639800	-2.18977500	1.33303900
H	2.27896800	-2.97660300	0.01594300
O	2.30680600	-0.31491300	1.53044200
H	3.22392400	-0.00259200	1.44252700
H	1.85294500	0.37506200	2.05657000
O	4.30802400	-0.14776900	-1.69743700
H	4.65237500	0.23879100	-0.86683200
H	4.94298500	0.03901900	-2.39568400
O	0.70278000	2.81435100	0.04815500
H	-0.12350400	3.31699000	-0.12926300

H	0.67479000	2.00331200	-0.49862400
O	-1.11902800	-3.23352600	-0.95007700
H	-0.72585600	-3.99028900	-0.48334500
H	-0.40665300	-2.72699400	-1.38613000
O	-4.63448600	0.12328600	-0.81147600
H	-4.46457300	1.07466000	-0.84754800
H	-4.49597200	-0.15222300	0.11446900
O	-4.12371500	-0.88157700	1.77569400
H	-3.42382100	-1.57113200	1.75748700
H	-4.89876200	-1.28138200	2.18176600
O	-0.11380900	-4.59411900	1.27618200
H	0.13961500	-5.47760900	1.55826800
H	0.72132200	-4.05084400	1.22542200
O	1.62333600	0.46170800	-1.04620100
H	1.77421700	0.06121300	-0.16374200
H	2.49212700	0.45420700	-1.48073300
O	-1.91937900	-2.45694700	1.55542600
H	-1.69173500	-2.53660900	0.60499700
H	-1.52188700	-3.26137300	1.92492900
O	0.25779300	-1.38879000	-2.47942200
H	0.56526200	-0.60794100	-1.97073100
H	-0.60469700	-1.16183400	-2.85798700
O	3.28784600	3.36861200	0.39136100
H	2.32845000	3.25900100	0.17774500
H	3.61997700	4.07759800	-0.16760000
O	2.71032300	-2.57905400	-1.67711700
H	1.94535700	-2.30487800	-2.20813600
H	3.34936400	-1.85125800	-1.72682600
O	1.07584500	1.93422400	2.57608600
H	1.58763800	2.58215000	3.07063600
H	0.87686700	2.33814900	1.69780700
O	4.63162100	1.10210400	0.71662600
H	4.16563400	1.97268100	0.59764500
H	5.40091600	1.26018300	1.27310000

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F(A)(W)<sub>19</sub>

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Coordination

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Symbol

C	-3.80488800	-0.91699800	0.98226600
O	-4.79791100	-0.79428500	0.30143000
H	-3.71744500	-1.67088700	1.77834700
O	-2.74365300	-0.14016900	0.84106400
H	-2.08431900	-0.17552600	1.62895200
N	-5.81149600	1.91745700	-0.82717100
H	-5.65115100	0.93109800	-0.61399300
H	-6.60649700	2.22522400	-0.27598400
H	-6.07597700	1.98661700	-1.80455300
O	1.40725100	-0.42333000	3.49046200
H	1.65383300	-0.16417300	4.38402200

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H	1.81236000	0.22026700	2.85881200
O	-1.16619600	2.79809000	1.98221800
H	-0.39130700	3.09423000	1.47534200
H	-1.94320400	2.99317500	1.43137200
O	-1.13585500	-2.33728300	-2.56452500
H	-0.28755800	-2.80132900	-2.55304100
H	-0.98097900	-1.44882500	-2.93202000
O	2.04708600	-2.83068300	2.18100400
H	1.90694500	-2.05570600	2.75364100
H	1.17613100	-3.04017500	1.79355300
O	1.65793700	-0.42368900	-2.14936000
H	1.04536100	-0.33209500	-1.37634900
H	1.17205500	-0.07697200	-2.91507600
O	-3.23416800	2.48544200	0.04964900
H	-3.21776600	1.56885100	0.38226500
H	-4.14772000	2.57046600	-0.31456900
O	5.19849800	2.27911000	-0.67777100
H	4.86765900	1.35974900	-0.64085800
H	5.82582400	2.38019000	0.04417200
O	-1.00032800	1.69614600	-1.26608600
H	-0.87615100	0.92867200	-0.66749700
H	-1.84120200	2.11947200	-0.98018100
O	0.17500500	-0.35101100	0.06852800
H	-0.05945200	-1.27395900	0.31803700
H	0.80388700	-0.00138700	0.72934200
O	3.75151300	-2.79630000	0.19874000
H	3.15131800	-2.79701900	1.00076900
H	4.50401300	-3.35828400	0.40930300
O	-0.64589600	0.30925000	-3.51490000
H	-0.90063100	0.93176700	-2.78861700
H	-1.04652100	0.62077300	-4.33181800
O	1.57921100	-3.11981100	-1.63026900
H	2.40353600	-3.34526900	-1.16693700
H	1.71955800	-2.19965200	-1.93458800
O	-0.14042700	-3.00944100	0.53274200
H	-1.06896600	-3.27202500	0.38337100
H	0.35628900	-3.19634800	-0.29253800
O	3.22922500	4.17669300	-0.89279500
H	3.95869200	3.52318000	-0.84206100
H	3.36883700	4.69817100	-1.68775400
O	-1.28724500	0.22007100	2.83648000
H	-1.16033800	1.18189400	2.65508300
H	-0.42328100	-0.14510200	3.09427800
O	-2.67472100	-3.03838900	-0.42221400
H	-3.46579900	-3.53181900	-0.65775200
H	-2.28044800	-2.70528700	-1.25689500
O	3.84148300	-0.11732500	-0.52669600
H	3.98499000	-1.05595900	-0.28632500
H	3.21025400	-0.13168400	-1.27473400
O	0.99463800	3.03426200	0.16004200

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H	0.41519300	2.66522700	-0.53523800
H	1.69427600	3.57214000	-0.26800100
O	2.19453600	0.98557000	1.41973400
H	1.82500900	1.81400800	1.02769700
H	2.88061600	0.65075400	0.80580000

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Table S2. ZPE-corrected binding energies ( $\Delta E_{\text{ZPE}}$ ) (in kcal/mol) for various isomers of  $\text{F}(\text{W})_n$  and  $\text{F}(\text{A})(\text{W})_{n-1}$  clusters ( $n=1-8, 10, 12, 14, 16, 18, 20$ ), and ZPE-corrected successive binding energies ( $\Delta E_{\text{ZPE},n}$ ) of  $\text{F}(\text{W})_n$  ( $n=1-8$ ) clusters at absolute zero temperature (0 K).

Cluster $\text{F}(\text{W})_n$	Functional	$\Delta E_{\text{ZPE}}$	$E_{\text{ZPE},n}$	Cluster $\text{F}(\text{A})(\text{W})_{n-1}$	Functional	$\Delta E_{\text{ZPE}}$
n=1	B3LYP	-10.91	-10.91	n=1	B3LYP	-15.57
	CAM-B3LYP	-12.51	-12.51		CAM-B3LYP	-13.83
	M06-2X	-12.84	-12.84		M06-2X	-14.45
	$\omega$ B97x-D	-11.94	-11.94		$\omega$ B97x-D	-14.10
n=2	B3LYP	-19.88	-8.97	n=2	B3LYP	-19.24
	CAM-B3LYP	-22.70	-10.18		CAM-B3LYP	-21.72
	M06-2X	-22.50	-9.66		M06-2X	-21.95
	$\omega$ B97x-D	-21.70	-9.76		$\omega$ B97x-D	-21.55
n=3	B3LYP	-25.90	-6.01	n=3	B3LYP	-22.74
	CAM-B3LYP	-29.70	-7.01		CAM-B3LYP	-25.99
	M06-2X	-28.70	-6.20		M06-2X	-26.46
	$\omega$ B97x-D	-27.75	-6.04		$\omega$ B97x-D	-25.74
n=4	B3LYP	-31.31	-5.42	n=4	B3LYP	-27.58
	CAM-B3LYP	-36.52	-6.82		CAM-B3LYP	-31.57
	M06-2X	-36.21	-7.51		M06-2X	-32.84
	$\omega$ B97x-D	-34.91	-7.16		$\omega$ B97x-D	-31.38
n=5	B3LYP	-36.84	-5.53	n=5	B3LYP	-33.99
	CAM-B3LYP	-43.18	-6.66		CAM-B3LYP	-39.59
	M06-2X	-44.09	-7.88		M06-2X	-40.65
	$\omega$ B97x-D	-41.88	-6.98		$\omega$ B97x-D	-39.30
n=6	B3LYP	-45.33	-8.48	n=6	B3LYP	-42.42
	CAM-B3LYP	-52.10	-8.92		CAM-B3LYP	-50.94
	M06-2X	-50.37	-6.28		M06-2X	-51.47
	$\omega$ B97x-D	-48.82	-6.93		$\omega$ B97x-D	-48.96
n=7	B3LYP	-50.64	-5.31	n=7	B3LYP	-52.51
	CAM-B3LYP	-60.48	-8.37		CAM-B3LYP	-61.42
	M06-2X	-62.31	-11.94		M06-2X	-62.72
	$\omega$ B97x-D	-59.45	-10.63		$\omega$ B97x-D	-60.95
n=8	B3LYP	-57.87	-7.22	n=8	B3LYP	-54.64
	CAM-B3LYP	-68.57	-8.09		CAM-B3LYP	-64.86
	M06-2X	-70.24	-7.92		M06-2X	-68.04
	$\omega$ B97x-D	-66.99	-7.54		$\omega$ B97x-D	-65.62
n=10	B3LYP	-71.38		n=10	B3LYP	-67.16
	CAM-B3LYP	-84.36			CAM-B3LYP	-79.14
	M06-2X	-83.48			M06-2X	-83.25
	$\omega$ B97x-D	-81.30			$\omega$ B97x-D	-79.51
n=12	B3LYP	-79.03		n=12	B3LYP	-77.28
	CAM-B3LYP	-98.45			CAM-B3LYP	-95.71
	M06-2X	-107.16			M06-2X	-104.27
	$\omega$ B97x-D	-100.69			$\omega$ B97x-D	-97.65
n=14	B3LYP	-99.02		n=14	B3LYP	-99.82
	CAM-B3LYP	-119.32			CAM-B3LYP	-116.72
	M06-2X	-121.48			M06-2X	-119.47
	$\omega$ B97x-D	-117.57			$\omega$ B97x-D	-115.74
n=16	B3LYP	-110.77		n=16	B3LYP	-115.62
	CAM-B3LYP	-134.39			CAM-B3LYP	-135.18
	M06-2X	-137.49			M06-2X	-138.21
	$\omega$ B97x-D	-132.69			$\omega$ B97x-D	-134.86
n=18	B3LYP	-124.32		n=18	B3LYP	-118.70
	CAM-B3LYP	-151.26			CAM-B3LYP	-145.87
	M06-2X	-156.05			M06-2X	-154.62
	$\omega$ B97x-D	-150.60			$\omega$ B97x-D	-147.42
n=20	B3LYP	-132.86		n=20	B3LYP	-133.91
	CAM-B3LYP	-164.12			CAM-B3LYP	-164.44
	M06-2X	-173.60			M06-2X	-173.01
	$\omega$ B97x-D	-165.78			$\omega$ B97x-D	-166.80

Method<sup>1</sup>: B3LYP/6-311++G(2d,2p)// B3LYP/6-31++G(d,p), Method<sup>2</sup>: CAM-B3LYP/6-311++G(2d,2p)// CAM-B3LYP/6-31++G(d,p),  
Method<sup>3</sup>: M06-2X/6-311++G(2d,2p)// M06-2X/6-31++G(d,p), Method<sup>4</sup>:  $\omega$ B97x-D/6-311++G(2d,2p)//  $\omega$ B97x-D/6-31++G(d,p),

F = HCOOH, A = NH<sub>3</sub>, W = H<sub>2</sub>O

Table S3. Binding energies ( $\Delta E_B$ ) (in kcal/mol), BSSE-corrected binding energies ( $\Delta E_{CP}$ ) (in kcal/mol) for various isomers of  $F(W)_n$  and  $F(A)(W)_{n-1}$  clusters ( $n= 1-8, 10, 12, 14, 16, 18, 20$ ), and successive binding energies ( $\Delta E_n$ ) of  $F(W)_n$  ( $n= 1-8$ ) clusters at temperature (298.15 K), and pressure (1013.25 hPa).

Cluster $F(W)_n$	Functional	$\Delta E_B$	$\Delta E_{CP}$	$\Delta E_n$	Cluster $F(A)(W)_{n-1}$	Functional	$\Delta E_B$	$\Delta E_{CP}$	$\Delta E_W$	$\Delta E_A$
n=1	B3LYP	-13.80	-13.30	-13.30	n=1	B3LYP	-14.95	-14.54		
	CAM-B3LYP	-15.52	-15.02	-15.02		CAM-B3LYP	-16.37	-15.95		
	M06-2X	-15.81	-15.28	-15.28		M06-2X	-16.80	-16.32		
	$\omega$ B97x-D	-15.15	-14.64	-14.64		$\omega$ B97x-D	-16.60	-16.23		
n=2	B3LYP	-25.16	-23.99	-11.36	n=2	B3LYP	-24.22	-23.22	-9.28	-10.42
	CAM-B3LYP	-28.16	-26.99	-12.63		CAM-B3LYP	-26.89	-26.14	-10.52	-11.37
	M06-2X	-27.58	-26.32	-11.77		M06-2X	-26.61	-25.47	-9.82	-10.80
	$\omega$ B97x-D	-23.15	-26.28	-8.00		$\omega$ B97x-D	-26.77	-25.80	-10.17	-11.62
n=3	B3LYP	-33.85	-32.14	-8.68	n=3	B3LYP	-30.07	-28.53	-5.85	-4.91
	CAM-B3LYP	-37.90	-36.19	-9.73		CAM-B3LYP	-33.60	-32.04	-6.71	-5.45
	M06-2X	-36.41	-34.58	-8.83		M06-2X	-33.65	-31.87	-7.01	-6.07
	$\omega$ B97x-D	-36.54	-34.83	-13.40		$\omega$ B97x-D	-33.58	-32.04	-6.81	-10.43
n=4	B3LYP	-43.09	-40.68	-9.24	n=4	B3LYP	-37.10	-35.63	-7.03	-3.25
	CAM-B3LYP	-48.57	-46.17	-10.68		CAM-B3LYP	-41.38	-39.28	-7.77	-3.49
	M06-2X	-47.02	-45.25	-10.61		M06-2X	-42.47	-40.06	-8.82	-6.06
	$\omega$ B97x-D	-47.64	-45.22	-11.09		$\omega$ B97x-D	-41.70	-39.58	-8.12	-5.16
n=5	B3LYP	-49.43	-46.51	-6.34	n=5	B3LYP	-45.93	-43.37	-8.83	-2.84
	CAM-B3LYP	-56.31	-53.41	-7.74		CAM-B3LYP	-52.14	-49.48	-10.77	-3.57
	M06-2X	-56.76	-53.64	-9.74		M06-2X	-52.41	-49.40	-9.94	-5.39
	$\omega$ B97x-D	-55.78	-52.81	-8.14		$\omega$ B97x-D	-52.21	-49.45	-10.51	-4.57
n=6	B3LYP	-58.77	-55.32	-9.34	n=6	B3LYP	-57.18	-53.72	-11.25	-7.74
	CAM-B3LYP	-66.27	-62.82	-9.96		CAM-B3LYP	-66.31	-62.92	-14.17	-10.00
	M06-2X	-64.04	-60.29	-7.30		M06-2X	-66.28	-62.45	-13.87	-9.52
	$\omega$ B97x-D	-63.90	-60.48	-8.12		$\omega$ B97x-D	-65.51	-61.69	-13.30	-9.73
n=7	B3LYP	-71.20	-66.82	-12.43	n=7	B3LYP	-70.85	-66.45	-13.67	-12.08
	CAM-B3LYP	-80.62	-76.24	-14.35		CAM-B3LYP	-80.40	-75.99	-14.09	-4.16
	M06-2X	-80.30	-75.63	-16.26		M06-2X	-80.65	-75.80	-14.37	-16.61
	$\omega$ B97x-D	-79.67	-75.12	-15.78		$\omega$ B97x-D	-80.46	-76.06	-14.95	-16.56
n=8	B3LYP	-80.50	-75.37	-9.30	n=8	B3LYP	-75.37	-70.44	-4.52	-4.17
	CAM-B3LYP	-91.43	-86.32	-10.81		CAM-B3LYP	-86.36	-81.43	-5.97	-5.75
	M06-2X	-91.11	-85.50	-10.80		M06-2X	-88.57	-83.06	-7.91	-8.27
	$\omega$ B97x-D	-90.57	-90.57	-10.89		$\omega$ B97x-D	-87.55	-82.55	-7.09	-7.88
n=10	B3LYP	-97.19	-90.38		n=10	B3LYP	-91.11	-84.44		
	CAM-B3LYP	-111.17	-104.57			CAM-B3LYP	-106.25	-99.77		
	M06-2X	-109.09	-101.87			M06-2X	-108.72	-101.65		
	$\omega$ B97x-D	-108.91	-102.22			$\omega$ B97x-D	-107.45	-100.90		
n=12	B3LYP	-112.78	-103.79		n=12	B3LYP	-108.98	-100.76		
	CAM-B3LYP	-133.13	-124.44			CAM-B3LYP	-128.49	-120.53		
	M06-2X	-140.41	-130.93			M06-2X	-135.51	-126.85		
	$\omega$ B97x-D	-136.02	-127.05			$\omega$ B97x-D	-131.43	-123.30		
n=14	B3LYP	-137.60	-127.40		n=14	B3LYP	-133.01	-123.36		
	CAM-B3LYP	-159.10	-149.20			CAM-B3LYP	-154.17	-144.82		
	M06-2X	-159.53	-148.65			M06-2X	-155.43	-145.21		
	$\omega$ B97x-D	-158.43	-148.33			$\omega$ B97x-D	-153.94	-144.43		
n=16	B3LYP	-155.08	-143.38		n=16	B3LYP	-155.75	-144.78		
	CAM-B3LYP	-180.02	-168.68			CAM-B3LYP	-180.11	-169.46		
	M06-2X	-181.06	-168.62			M06-2X	-181.20	-170.35		
	$\omega$ B97x-D	-179.52	-167.94			$\omega$ B97x-D	-183.44	-172.75		
n=18	B3LYP	-173.77	-160.32		n=18	B3LYP	-166.88	-153.92		
	CAM-B3LYP	-202.20	-189.17			CAM-B3LYP	-195.53	-182.97		
	M06-2X	-204.53	-190.30			M06-2X	-202.37	-188.65		
	$\omega$ B97x-D	-203.14	-189.82			$\omega$ B97x-D	-198.37	-185.51		
n=20	B3LYP	-188.03	-172.98		n=20	B3LYP	-188.90	-174.41		
	CAM-B3LYP	-220.84	-206.28			CAM-B3LYP	-221.11	-207.07		
	M06-2X	-228.15	-212.25			M06-2X	-227.12	-211.75		
	$\omega$ B97x-D	-224.17	-209.20			$\omega$ B97x-D	-225.03	-210.65		

Method<sup>1</sup>: B3LYP/6-311++G(2d,2p)// B3LYP/6-31++G(d,p), Method<sup>2</sup>: CAM-B3LYP/6-311++G(2d,2p)// CAM-B3LYP/6-31++G(d,p),  
Method<sup>3</sup>: M06-2X/6-311++G(2d,2p)// M06-2X/6-31++G(d,p), Method<sup>4</sup>:  $\omega$ B97x-D/6-311++G(2d,2p)//  $\omega$ B97x-D/6-31++G(d,p),

F = HCOOH, A = NH<sub>3</sub>, W = H<sub>2</sub>O, and  $\Delta E_W: E_{F(W)_n(A)} - E_{F(W)_{n-1}(A)}$ ,  $\Delta E_A: E_{F(W)_n(A)} - E_{F(W)_n}$

Table S4. Binding enthalpies ( $\Delta H_B$ ) (in kcal/mol) for various isomers of  $F(W)_n$  and  $F(A)(W)_{n-1}$  clusters ( $n= 1-8, 10, 12, 14, 16, 18, 20$ ), and successive binding enthalpies ( $\Delta H_n$ ) of  $F(W)_n$  clusters at M06-2X/6-311++G(2d,2p) level of theory at temperature (298.15 K), and pressure (1013.25 hPa).

Cluster $F(W)_n$	$\Delta H_B$	$\Delta H_n$	Cluster $F(A)(W)_{n-1}$	$\Delta H_B$	$\Delta H_W$	$\Delta H_A$
n=1	-13.77	-13.77	n=1	-15.26		
n=2	-24.01	-10.24	n=2	-23.62	-8.36	-9.85
n=3	-31.20	-7.20	n=3	-28.84	-5.22	-4.83
n=4	-39.72	-8.52	n=4	-35.96	-7.12	-4.76
n=5	-47.41	-7.70	n=5	-44.40	-8.44	-4.68
n=6	-54.09	-6.67	n=6	-56.38	-11.98	-8.96
n=7	-67.57	-13.49	n=7	-68.89	-12.51	-18.51
n=8	-76.10	-8.53	n=8	-74.65	-7.08	-5.76
n=10	-92.02		n=10	-91.51		
n=12	-118.07		n=12	-114.63		
n=14	-134.09		n=14	-131.77		
n=16	-151.96		n=16	-152.10		
n=18	-172.09		n=18	-170.23		
n=20	-191.61		n=20	-190.45		

$$F = \text{HCOOH}, A = \text{NH}_3, W = \text{H}_2\text{O}, \Delta H_W: H_{F(W)_n(A)} - H_{F(W)_{n-1}(A)}, \Delta H_A: H_{F(W)_n(A)} - H_{F(W)_n}$$

Table S5. Calculated binding enthalpies,  $\Delta H_B$  of the  $F(W)_n$  clusters ( $n = 1-8, 10, 12, 14, 16, 18, 20$ ) (in kcal/mol) at the M06-2X/6-311++G(2d,2p)//M06-2X/6-31++G(d,p) level of theory at various temperature (T) and pressure (P).

T (K)	P (hPa)	Number of water molecules n													
		1	2	3	4	5	6	7	8	10	12	14	16	18	20
216.65	226.32	-13.80	-24.08	-31.22	-39.68	-47.65	-54.38	-67.76	-76.30	-91.85	-	-	-	-	-
226.75	287	-13.79	-24.09	-31.24	-39.71	-47.65	-54.37	-67.78	-76.32	-91.93	-	-	-	-	-
236.65	360	-13.79	-24.08	-31.25	-39.73	-47.64	-54.36	-67.78	-76.32	-91.99	-	-	-	-	-
246.55	446	-13.79	-24.07	-31.25	-39.75	-47.62	-54.34	-67.78	-76.32	-92.04	-	-	-	-	-
256.45	549	-13.79	-24.07	-31.25	-39.75	-47.59	-54.30	-67.75	-76.30	-92.06	-	-	-	-	-
266.35	670	-13.79	-24.06	-31.25	-39.75	-47.56	-54.26	-67.73	-76.27	-92.07	-	-	-	-	-
276.25	812	-13.78	-24.04	-31.23	-39.75	-47.52	-54.21	-67.69	-76.22	-92.07	-	-	-	-	-
286.15	977	-13.78	-24.03	-31.22	-39.74	-47.48	-54.16	-67.64	-76.18	-92.05	-	-	-	-	-
298.15	1013.25	-13.77	-24.01	-31.20	-39.72	-47.41	-54.09	-67.57	-76.10	-92.02	-	-	-	-	-

Table S6. Calculated binding enthalpies,  $\Delta H_B$  of the  $F(A)(W)_{n-1}$  clusters ( $n = 1-8, 10, 12, 14, 16, 18, 20$ ) (in kcal/mol) at the M06-2X/6-311++G(2d,2p)//M06-2X/6-31++G(d,p) level of theory at various temperature (T) and pressure (P).

T (K)	P (hPa)	Number of water molecules n													
		1	2	3	4	5	6	7	8	10	12	14	16	18	20
216.65	226.32	-15.30	-23.66	-28.89	-36.08	-44.50	-56.42	-68.80	-74.69	-91.49	-	-	-	-	-
226.75	287	-15.30	-23.66	-28.90	-35.67	-44.51	-56.45	-68.85	-74.73	-91.55	-	-	-	-	-
236.65	360	-15.29	-23.66	-28.90	-36.08	-44.52	-55.91	-68.89	-74.76	-91.68	-	-	-	-	-
246.55	446	-15.29	-23.66	-28.90	-36.08	-44.01	-56.48	-68.92	-74.77	-91.62	-	-	-	-	-
256.45	549	-15.29	-23.66	-28.90	-36.07	-45.00	-55.89	-68.93	-74.77	-91.63	-	-	-	-	-
266.35	670	-15.28	-23.66	-28.89	-36.05	-44.49	-56.46	-68.94	-74.76	-91.62	-	-	-	-	-
276.25	812	-15.28	-23.65	-28.88	-36.03	-44.47	-56.44	-68.93	-74.73	-91.60	-	-	-	-	-
286.15	977	-14.14	-22.75	-27.97	-35.11	-43.55	-55.53	-68.02	-73.81	-90.67	-	-	-	-	-
298.15	1013.25	-15.26	-23.62	-28.84	-35.96	-44.40	-56.38	-68.89	-74.65	-91.51	-	-	-	-	-

Table S7. Calculated successive free energy,  $\Delta G_n$  of the  $F(W)_n$  clusters ( $n = 1-8$ ) (in kcal/mol) at the M06-2X/6-311++G(2d,2p)//M06-2X/6-31++G(d,p) level of theory at various temperature (T) and pressure (P).

T (K)	P (hPa)	Number of water molecules n							
		1	2	3	4	5	6	7	8
216.65	226.32	-6.18	-3.22	0.66	-0.38	-2.14	-0.86	-2.67	-1.99
226.75	287	-5.94	-3.00	0.92	-0.11	-1.97	-0.70	-2.28	-1.79
236.65	360	-5.70	-2.78	1.16	0.15	-1.82	-0.54	-1.90	-1.60
246.55	446	-5.47	-2.57	1.41	0.40	-1.67	-0.39	-1.52	-1.42
256.45	549	-5.24	-2.37	1.65	0.66	-1.53	-0.24	-0.15	-1.08
266.35	670	-5.01	-2.17	1.88	0.90	-1.39	-0.09	-0.78	-1.06
276.25	812	-4.80	-1.98	2.11	1.14	-1.26	-0.04	-0.42	-0.89
286.15	977	-4.59	-1.80	2.33	1.38	-1.14	0.17	-0.06	-0.73
298.15	1013.25	-4.21	-1.45	2.72	1.78	-0.88	0.45	0.49	-0.41

Table S8. The mean isotropic ( $\bar{\alpha}$ ), anisotropic ( $\Delta\alpha$ ) polarizabilities and Rayleigh scattering intensities ( $\mathfrak{R}_n$ ) of HCOOH, H<sub>2</sub>O, and NH<sub>3</sub> are calculated at the CAM-B3LYP/aug-cc-pVDZ level of theory at the static frequency ( $\infty$ ).

Molecule	$\bar{\alpha}$ (a.u.)	$\Delta\alpha$ (a.u.)	$\mathfrak{R}_n$ (a.u.)
HCOOH	22.4635	12.5219	22870.18215
NH <sub>3</sub>	13.9611	1.48729	8790.388864
H <sub>2</sub> O	9.31205	1.129	3916.819384

Table S9. The mean isotropic ( $\bar{\alpha}$ ), anisotropic ( $\Delta\alpha$ ) polarizabilities, and Rayleigh scattering intensities ( $\mathfrak{R}_n$ ) of  $F(W)_n$  and  $F(A)(W)_{n-1}$  ( $n = 1-8, 10, 12, 14, 16, 18, 20$ ) clusters are calculated at the CAM-B3LYP/aug-cc-pVDZ level of theory at the static frequency ( $\infty$ ). The calculated ( $\bar{\alpha}$ ), ( $\Delta\alpha$ ), and  $\mathfrak{R}_n$  are given in atomic units (a.u.).

$F(W)_n$			$F(A)(W)_{n-1}$				
n	$\bar{\alpha}$ (a.u.)	$\Delta\alpha$ (a.u.)	$\mathfrak{R}_n$ (a.u.)	n	$\bar{\alpha}$ (a.u.)	$\Delta\alpha$ (a.u.)	$\mathfrak{R}_n$ (a.u.)
1	31.45	12.48	44671.85	1	36.19	14.25	59122.47
2	42.02	16.40	79668.82	2	46.44	17.86	97282.49
3	51.93	18.87	121597.93	3	56.01	17.07	141392.31
4	61.2	15.13	168741.49	4	64.77	17.06	189003.66
5	70.50	9.83	223789.04	5	74.94	15.18	252917.50
6	82.32	25.65	305279.66	6	85.03	49.31	325995.57
7	90.08	12.40	365309.49	7	94.63	16.48	403181.90
8	100.50	20.31	454775.28	8	103.70	20.61	484183.98
10	120.67	18.14	839221.22	10	123.45	29.17	686174.82
12	136.55	11.97	843169.40	12	142.81	34.51	918209.95
14	158.19	13.89	1126263.95	14	161.92	18.84	1180058.81
16	177.11	21.77	141840.86	16	182.10	28.01	1492582.58
18	195.91	12.00	1727288.77	18	200.80	29.42	1814811.26
20	213.76	14.51	2056388.82	20	219.95	37.08	2177096.26

F = HCOOH, A = NH<sub>3</sub>, W = H<sub>2</sub>O