Supplementary Information

Structures, Energetics and Vibrational Spectra of (H₂O)₃₂ Clusters: A Journey from Model Potentials to Correlated Theory

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Fragmentation details for the W32-TIP4P-Ew isomer. The monomer indices only for the main fragments are listed below. Size indicates the number of water monomers in each main fragment.

W32-TIP4P-Ew Isomer

Main Fragments = 29; # Overlap Fragments = 135; # Total Fragments = 164

Average size of Fragments = 28.55; R-goodness = 3.61 Å

Fragment Number	Size	Monomer Indices												
1	13	2	6	7	12	13	14	18	19	27	29	30	31	32
2	11	1	2	12	13	16	17	18	19	20	25	27		
3	11	2	3	7	12	13	17	18	19	20	24	25		
4	11	1	6	12	13	18	19	25	27	29	31	32		
5	13	2	6	7	11	12	13	16	18	19	27	30	31	32
6	12	2	3	7	12	13	14	16	18	19	20	22	25	
7	10	1	2	12	13	15	16	17	18	19	27			
8	11	1	10	12	13	17	18	19	25	27	29	31		
9	11	2	6	7	11	12	13	16	19	21	28	30		
10	11	2	6	7	11	13	14	18	23	30	31	32		
11	11	3	4	7	12	17	19	20	22	24	25	26		
12	10	1	6	10	12	13	18	27	29	31	32			
13	9	2	4	12	13	16	17	19	21	27				
14	9	1	5	12	18	19	24	25	26	31				
15	8	5	13	14	18	23	25	30	31					
16	10	6	8	10	12	13	15	17	18	27	29			
17	9	2	3	7	9	13	14	19	30	22				
18	9	1	12	15	17	18	19	20	26	27				
19	11	2	6	8	11	13	18	27	28	29	30	32		
20	9	2	4	7	12	13	16	19	21	28				
21	9	1	10	12	15	17	18	25	29	27				
22	9	3	5	7	9	13	14	19	30	31				
23	9	1	6	10	13	15	18	27	29	32				
24	6	5	9	14	24	25	31							
25	7	6	8	11	13	21	27	32						
26	8	6	11	13	18	23	29	30	32					
27	7	2	6	8	12	16	21	28						
28	5	4	12	16	19	20								
29	7	5	19	20	22	24	25	26						

Grafting details for W32-TIP4P-Ew isomer at MP2/aug-cc-pvDZ and MP2/aug-cc-pvTZ levels of theory, employing the above fragmentation scheme.

(i) MTA-Calculations:

MP2/6-31+G* : E = -2439.406029 A.U. and E2 = -6.3958969 A.U.

MP2/aug-cc-pvDZ: E = -2440.924821 A.U. and E2 = -7.2778702 A.U.

MP2/aug-cc-pvTZ: E = -2443.086057 A.U.

(ii) Full Calculations:

MP2/6-31+G* : E = -2439.431602 A.U. and E2 = -6.397706 A.U.

MP2/aug-cc-pvDZ: E = -2440.952431 A.U.

HF/aug-cc-pvDZ : E = -2433.672302 A.U.

(iii) Grafted Energies:

GE-MP2/aug-cc-pvDZ = -2440.951981 A.U.

GE-MP2/aug-cc-pvTZ = -2443.113667 A.U.

Cartesian atomic coordinates (in Å) for W32-AMOEBA, W32-TTM2.1_F, W32-TIP4P/2005, W32-TIP4P, W32-TIP4P-Ew, W32-T1, W32-T7, W32-G1 and W32-G2 isomers. The isomers are being optimized at MP2/aug-cc-pvDZ level of theory within MTA.

W32-AMOEBA

8	0.855365400	-3.271158100	-0.075797300
1	1.118860900	-2.326280300	-0.054274400
1	1.022589500	-3.614846300	0.825456600
8	-1.672087400	-3.133050300	-1.197174600
1	-0.817511600	-3.318409900	-0.748793200
1	-1.563467700	-3.507157600	-2.095985600
8	1.716354000	-0.628025600	-0.180534200
1	2.097728500	-0.545256200	-1.088614200
1	1.150527300	0.173221400	-0.099080500
8	1.150637700	-4.135224400	2.581058000
1	1.695354900	-3.515564400	3.122839500
1	1.480314200	-5.019351300	2.786514000
8	1.608515500	-4.436952100	-2.561767200
1	1.450741400	-4.127202800	-1.649276900
1	0.712722900	-4.546608800	-2.935721500
8	-1.420698000	-2.850304900	2.699495200
1	-0.673867000	-3.474672700	2.728653300
1	-1.058926100	-2.054681900	2.240023200
8	-1.441742900	-0.425708500	-1.055078400
1	-1.592301900	-1.393813200	-1.185184700

1	-1.098687900	-0.372012800	-0.134007700
8	-0.837293200	-0.420309300	1.648885100
1	-0.120227500	0.093562200	2.088364000
1	-1.653194600	-0.037245300	2.047242200
8	-0.972654300	-4.112303800	-3.716443600
1	-0.679427900	-3.333494900	-4.259565900
1	-1.529148700	-4.649170100	-4.294403600
8	3.258370200	-0.240657400	2.009850500
1	2.808499800	-0.483261600	1.162575100
1	3.894602100	0.448728100	1.741408400
8	2.547180600	-0.224439800	-2.739800600
1	2.749326300	-1.042566800	-3.239110800
1	1.667536100	0.057257500	-3.075221500
8	2.513708000	-2.223745700	3.972623600
1	2.946669800	-1.583723900	3.379298400
1	1.917565300	-1.687143600	4.527165000
8	-3.649581600	-2.857874700	0.879515300
1	-3.134802800	-3.027583100	0.069591300
1	-2.993565700	-3.009384100	1.585047300
8	2.726141600	-2.614598000	-4.171664400
1	2.418762200	-3.339804300	-3.565493600
1	3.510602700	-2.953272200	-4.620294200
8	-0.090814800	0.337754200	-3.363782000
1	-0.546612500	0.130906300	-2.520029900
1	-0.400923800	1.229755100	-3.622358600
8	0.467838100	1.837781000	0.013216100
1	-0.429009700	2.013520800	0.382377500
1	1.056965000	2.324874100	0.635285100
8	0.068806000	-1.998095000	-4.983949500
1	1.031654900	-2.146033800	-4.912087100
1	-0.076735500	-1.144446800	-4.532369400
8	1.105909500	0.983872800	3.099388000
1	1.928053500	0.530757900	2.778848100
1	0.977774800	0.633939000	4.007441900
8	-1.892537600	-1.119240700	4.859315800
1	-1.817344300	-1.848559100	4.208099800
1	-2.361842600	-0.423621100	4.365127200
8	0.651177700	-0.495076100	5.400476700
1	-0.307460300	-0.729567900	5.262854300
1	0.740505800	-0.319483200	6.345362300
8	-3.058952700	0.693913900	2.848758100
1	-3.836160400	0.390462500	2.340039900
1	-2.819010200	1.557447900	2.453913600

8	3.836418900	2.141423500	-1.719760800
1	3.589015900	1.284575200	-2.113393700
1	3.072630900	2.706051700	-1.940696700
8	-3.528738400	1.277769700	-0.793673500
1	-2.840017800	0.604388100	-1.020568900
1	-4.209492300	0.759342500	-0.324821100
8	-4.913663700	-0.463715600	1.043417300
1	-4.495009800	-1.358336900	0.961493600
1	-5.853133100	-0.638636800	1.184256800
8	4.478259200	2.134266800	0.915481000
1	4.294267200	2.128487600	-0.058384400
1	5.367537100	2.501659100	1.000337600
8	-2.029821500	2.561093200	1.057407800
1	-2.629449500	2.159983400	0.376337800
1	-2.061382700	3.523511400	0.867631600
8	2.028023700	3.261701300	1.789608100
1	1.715788200	2.674875400	2.509020800
1	2.953949000	2.994230700	1.628844500
8	1.274476400	3.411469300	-2.041425000
1	0.877948700	2.748900100	-1.425982100
1	0.695021300	3.393304200	-2.824089100
8	-0.850048400	2.982048700	-3.933323000
1	-1.632277200	3.273577000	-3.406611300
1	-1.024144200	3.269234000	-4.838659900
8	-2.893339300	3.680619300	-2.264532500
1	-3.290459500	2.902402400	-1.832836900
1	-2.583686700	4.242755400	-1.530394700
8	0.810254200	5.271647600	0.009960600
1	1.228594300	4.771386600	0.732955600
1	1.057795900	4.762690000	-0.790971200
8	-1.860743000	5.135369800	0.040673700
1	-0.870726100	5.250193300	0.038085800
1	-2.218869800	5.991315000	0.305583300

W32-TTM2.1_F

8	-3.323660000	0.676650000	1.789430000
1	-3.243550000	0.774490000	2.760090000
1	-2.549590000	1.161060000	1.425560000
8	-2.733840000	0.825160000	4.542620000
1	-1.776430000	0.625940000	4.593400000
1	-3.153770000	0.164600000	5.108670000
8	-1.086420000	1.807500000	0.640390000
1	-1.273830000	2.153740000	-0.263970000

1	-0.558490000	2.517500000	1.070050000
8	-2.793540000	-1.837790000	0.792260000
1	-3.059010000	-1.014780000	1.257810000
1	-3.580320000	-2.108770000	0.282750000
8	-5.133400000	0.647600000	-0.446340000
1	-4.648680000	0.703710000	0.397830000
1	-5.126990000	-0.299910000	-0.675650000
8	0.597860000	-0.090090000	1.730750000
1	0.035650000	0.502950000	1.183130000
1	0.372240000	0.162310000	2.654670000
8	-1.143890000	-0.885630000	-1.275790000
1	-1.702260000	-1.148730000	-0.510770000
1	-0.906800000	-1.749490000	-1.700080000
8	-4.926690000	-2.194010000	-1.022570000
1	-4.403340000	-2.439410000	-1.827430000
1	-5.690860000	-2.784420000	-1.022320000
8	0.093530000	0.550470000	4.389150000
1	0.556130000	1.404600000	4.494100000
1	0.706360000	-0.114170000	4.761770000
8	-0.178700000	-2.727630000	1.432120000
1	-1.146760000	-2.676810000	1.326940000
1	0.090660000	-1.785380000	1.497530000
8	-1.546470000	2.979410000	-1.779530000
1	-2.432570000	2.803040000	-2.147370000
1	-0.883380000	2.731300000	-2.468480000
8	-4.125470000	2.054570000	-2.514180000
1	-4.531420000	1.599010000	-1.730750000
1	-4.846750000	2.542800000	-2.930720000
8	0.769890000	3.604190000	1.634410000
1	1.088470000	3.473620000	2.548470000
1	1.481900000	3.233200000	1.063620000
8	-2.503540000	-0.031460000	-3.485200000
1	-2.062170000	-0.194730000	-2.616800000
1	-3.135200000	0.692880000	-3.311050000
8	1.235270000	0.465150000	-1.425850000
1	0.359730000	0.063030000	-1.227580000
1	1.797650000	-0.319040000	-1.623650000
8	-3.397950000	-2.696030000	-3.181060000
1	-3.173570000	-1.788500000	-3.474560000
1	-2.528990000	-3.098140000	-3.006020000
8	1.743140000	2.858610000	4.233790000
1	2.517390000	2.235570000	4.238070000
1	1.933850000	3.511860000	4.919090000

8	0.007120000	5.102650000	-0.701160000
1	-0.714260000	4.528340000	-1.024580000
1	0.154730000	4.820970000	0.220060000
8	-0.564140000	-3.210400000	-2.582710000
1	0.013620000	-3.728070000	-1.989620000
1	0.021070000	-2.954640000	-3.329500000
8	1.892100000	-3.389210000	3.300870000
1	1.054940000	-3.336030000	2.808110000
1	2.548130000	-3.655100000	2.625670000
8	2.522370000	2.539080000	-0.184210000
1	2.019400000	1.814310000	-0.616750000
1	2.647550000	3.205130000	-0.888140000
8	3.327730000	0.379760000	1.419400000
1	2.359760000	0.203440000	1.481150000
1	3.366660000	1.197130000	0.887960000
8	2.126800000	-1.334620000	5.016440000
1	2.091360000	-2.097340000	4.380750000
1	2.286360000	-1.742830000	5.877410000
8	1.316580000	-3.861520000	-0.575360000
1	0.761970000	-3.478900000	0.140390000
1	2.088510000	-4.219420000	-0.091400000
8	0.595640000	2.303640000	-3.337480000
1	0.937070000	1.620040000	-2.715100000
1	1.195870000	3.065030000	-3.211090000
8	3.633820000	0.937530000	4.163200000
1	3.699400000	0.746900000	3.205900000
1	3.242630000	0.117650000	4.524660000
8	-0.176870000	0.124020000	-4.996320000
1	-1.072540000	0.113680000	-4.596260000
1	0.206440000	0.955180000	-4.658420000
8	2.572690000	-1.863910000	-2.050340000
1	2.104350000	-2.574790000	-1.555850000
1	2.296170000	-1.980300000	-2.978490000
8	2.093970000	4.433160000	-2.234150000
1	1.346060000	4.792970000	-1.681890000
1	2.563360000	5.201280000	-2.580810000
8	4.436610000	-1.803860000	0.090390000
1	4.107000000	-1.016640000	0.580420000
1	4.014660000	-1.732610000	-0.784490000
8	1.125960000	-2.114190000	-4.481880000
1	0.664960000	-1.251400000	-4.698460000
1	1.356920000	-2.499160000	-5.336760000
8	3.552800000	-4.088780000	1.111860000

1	3.959010000	-3.244330000	0.762050000
1	4.285590000	-4.708930000	1.211720000

W32-TIP4P/2005

8	-2.434437100	-1.803302400	2.209835900
1	-1.857252000	-1.186449700	2.718001800
1	-2.157280300	-2.698161600	2.481525200
8	0.102856600	4.274581900	3.130443900
1	-0.300968700	4.732359000	2.371756800
1	0.918059400	3.863054400	2.775605000
8	1.294228800	-0.039021500	-1.283865100
1	1.345296700	0.845866900	-1.726085100
1	2.209736200	-0.385002000	-1.393310500
8	4.675243700	2.174190800	0.493255500
1	3.918288900	2.533572100	1.003230300
1	4.767083700	1.258619800	0.807533300
8	-3.387710400	4.219248000	0.021330600
1	-3.428683200	3.509140200	0.695292900
1	-3.298236900	3.729066800	-0.814854200
8	0.520850500	3.509848100	-0.360121500
1	-0.076215900	2.733179300	-0.248534400
1	-0.022267900	4.285400600	-0.109992500
8	4.363510000	2.028754500	-2.190754300
1	4.509883600	2.197770600	-1.224940400
1	5.085289900	2.480163000	-2.647974100
8	-1.201422700	1.384253800	-0.135889600
1	-1.037034600	0.416641100	-0.182667700
1	-1.821167600	1.580260800	-0.881833300
8	-0.383916100	-1.036673000	-3.245250000
1	0.191138900	-0.793043600	-2.481351100
1	0.023440200	-1.843116400	-3.617304200
8	2.236687000	2.933326200	1.753681700
1	1.978913500	1.986273200	1.798194400
1	1.758851500	3.217814500	0.946533300
8	4.921322700	-0.728736200	1.028587000
1	5.770307800	-1.096497100	1.304817500
1	4.247809800	-1.226599200	1.542035000
8	-4.485286800	-0.200002300	0.947522200
1	-3.966684000	-0.904957700	1.376008000
1	-4.116509400	0.617019600	1.344849200
8	3.966299200	-0.737522900	-1.634183900
1	4.236069100	0.129991100	-1.998704200
1	4.409985000	-0.784827100	-0.763841200

8	-1.079170300	-1.410118100	-0.111601100
1	-1.582836900	-1.587579100	0.720936100
1	-1.695276500	-1.699565900	-0.821686400
8	-0.597452600	-0.126861800	3.313013800
1	0.037942900	0.112896100	2.597224900
1	-0.866696800	0.724195900	3.717349600
8	-0.926844200	1.645588600	-4.026457100
1	-0.085051000	2.046255600	-3.749149000
1	-0.738383500	0.689050400	-3.951881400
8	-1.430314800	-4.577974700	-2.172911100
1	-0.720134200	-4.302700800	-2.782379200
1	-2.060403100	-3.831504900	-2.199519500
8	-1.514676800	2.390701100	4.124320000
1	-1.780388600	2.622203800	5.023354400
1	-0.913507600	3.124299200	3.823689300
8	0.683237000	-3.567866100	-3.856309100
1	0.875757500	-3.987351300	-4.704219500
1	1.550558000	-3.527996400	-3.367972200
8	0.831125800	-2.480800600	4.012470200
1	0.320859000	-1.645821200	3.977072000
1	0.218165900	-3.144356000	3.652333300
8	-1.108147000	5.459125800	0.754593700
1	-2.003077600	5.126333400	0.484853200
1	-1.138933800	6.419521400	0.658912200
8	1.359050600	0.297514300	1.468727700
1	1.227972400	0.209580900	0.497376800
1	1.929061000	-0.467906700	1.704269700
8	-3.050399800	2.040081100	1.779771500
1	-2.278683600	1.757324600	1.238101500
1	-2.685153000	2.190280900	2.674639000
8	-2.724223800	-2.055419700	-2.277877900
1	-2.018731300	-1.568913000	-2.759852400
1	-3.474205700	-1.431868400	-2.186605300
8	2.747867900	-2.037062300	2.094496900
1	2.196855600	-2.242616100	2.889297300
1	2.278705000	-2.495732500	1.368913500
8	1.205806900	-2.950216000	-0.048328500
1	0.442842900	-2.326462100	-0.125889300
1	0.774982500	-3.819578000	0.071546200
8	2.811095400	-3.317842600	-2.259996900
1	2.282169700	-3.159400800	-1.446599900
1	3.352153000	-2.510779300	-2.322461600
8	-0.367691000	-5.277915900	0.206349000

1	-0.028380000	-6.176811300	0.105083500
1	-0.833835600	-5.074319700	-0.646229100
8	-1.157470400	-4.293633600	2.725820100
1	-0.945056700	-4.706857800	1.862957900
1	-1.570165900	-4.995011500	3.245949100
8	-4.596498300	-0.088833800	-1.700783100
1	-4.588332400	-0.133788400	-0.702967600
1	-5.530412600	-0.104398900	-1.947742500
8	1.553423700	2.357258000	-2.596985500
1	2.527699000	2.414143100	-2.625858200
1	1.272636600	3.002129000	-1.913749400
8	-2.899265800	2.155620100	-2.112783100
1	-3.571728300	1.446543000	-2.154350800
1	-2.315943800	2.034998300	-2.893175000

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8	-3.435584800	1.071033100	1.364724800
1	-3.241606400	0.116060200	1.214852000
1	-3.440675600	1.168335600	2.338054300
8	-0.970752000	1.888677000	0.550821800
1	-1.893169500	1.715087700	0.856882700
1	-0.464816800	1.102347700	0.851670500
8	-2.786478700	-1.446915700	0.601645900
1	-2.177713400	-1.155433400	-0.123323100
1	-3.591326500	-1.761794200	0.139159300
8	-2.913232600	1.208320600	4.029089500
1	-1.953668900	1.098937600	4.196280000
1	-3.337778700	1.135528900	4.890916500
8	-4.899084300	0.970634700	-1.032603800
1	-4.545005300	1.137931200	-0.139453400
1	-5.019970400	0.006015300	-1.077570800
8	-1.062124100	-0.813162300	-1.395109900
1	-0.189988700	-0.369854500	-1.265575700
1	-0.849295600	-1.721810600	-1.720336800
8	0.494416300	-0.070171500	1.818139700
1	0.217340000	0.261775100	2.706998100
1	0.104516100	-0.977954800	1.774579600
8	-4.936602400	-1.888284300	-1.068633800
1	-4.422848800	-2.198900600	-1.858384900
1	-5.755465100	-2.399188200	-1.072707300
8	-0.187044700	0.890291600	4.278950200
1	0.304491400	1.744968500	4.288404400
1	0.347841400	0.290342200	4.836431500

8	-0.595033800	-2.541295200	1.770204600
1	-1.513116100	-2.359905200	1.472983800
1	-0.154164300	-2.997000800	1.019496500
8	-1.081219100	2.909727100	-1.989386700
1	-1.053944800	2.419350200	-1.139959400
1	-1.975203600	2.758052600	-2.351231800
8	-3.570891600	2.191461700	-2.994475700
1	-4.104263700	1.769883500	-2.271714200
1	-4.179711300	2.770981600	-3.468676400
8	0.896113000	3.668999300	1.344159000
1	0.116967700	3.088517700	1.172219500
1	1.094005200	3.562282200	2.293189100
8	-2.275694200	-0.160771300	-3.720096600
1	-1.855975900	-0.256576700	-2.832560500
1	-2.776708800	0.674037900	-3.657137400
8	1.376922600	0.356674300	-1.427311400
1	1.849974400	0.969198300	-0.820205700
1	1.302489400	0.879482300	-2.259553300
8	1.487531600	3.016809000	4.010190300
1	2.256892400	2.379623800	4.039912800
1	1.720191600	3.744214000	4.601166800
8	-3.389001600	-2.635420400	-3.123465100
1	-3.102381000	-1.790974700	-3.525875300
1	-2.552052300	-3.073497400	-2.886025800
8	0.660278400	4.939816300	-1.166810900
1	-0.086054400	4.391007400	-1.480622500
1	0.717297800	4.734992400	-0.216437500
8	-0.713064400	-3.316067200	-2.355051600
1	-0.271649800	-3.789200700	-1.622255500
1	-0.050995300	-3.287249300	-3.070561200
8	1.642262400	-0.909157700	5.369703300
1	1.577700400	-1.706026300	4.782274600
1	1.755544500	-1.259231500	6.261569000
8	2.807646200	2.232824100	-0.017044400
1	2.192601100	2.806271100	0.489592600
1	3.057671900	2.766285400	-0.797741800
8	0.924483600	-3.756498600	-0.171130700
1	1.517382200	-3.141411300	-0.654830400
1	1.522213100	-4.195884300	0.469487700
8	1.312732900	-3.006026300	3.759553100
1	0.510176400	-2.919934800	3.211690000
1	1.932658800	-3.504523600	3.196771200
8	3.193281900	0.047467600	1.620335700

1	2.209247800	-0.066294900	1.680950800
1	3.293568200	0.821589600	1.030457400
8	1.018429700	2.036957000	-3.556594400
1	0.226221100	2.402370900	-3.113450300
1	1.730828200	2.670265400	-3.346089000
8	3.270945900	1.064989300	4.163590900
1	2.848559600	0.342961900	4.664264000
1	3.417465700	0.674354300	3.272970700
8	2.496141300	-2.107676400	-1.724481100
1	2.179526900	-1.183177200	-1.634549900
1	2.276686100	-2.350277600	-2.645731700
8	0.220949800	-0.314198000	-4.900941000
1	-0.716264100	-0.240291000	-4.627926200
1	0.612351500	0.522463100	-4.596071700
8	1.310972500	-2.644176600	-4.168386900
1	0.931298300	-1.781014600	-4.482362400
1	1.572131100	-3.121480500	-4.965348700
8	2.787345900	3.806862500	-2.322789200
1	2.043569200	4.338310500	-1.931583400
1	3.405182900	4.448734300	-2.694430800
8	2.839631100	-4.321618100	1.758882800
1	3.397058000	-3.589872300	1.372609100
1	3.445185900	-5.057484900	1.910963100
8	4.122537000	-2.326594900	0.563627900
1	3.896750500	-1.459221700	0.968631000
1	3.757933500	-2.267580600	-0.337777600

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8	0.747076600	1.656420700	3.173748200
1	1.363550700	2.208937400	2.645779600
1	0.169458900	2.292371600	3.635194900
8	0.048168500	-0.956352400	-3.101531200
1	-0.541744500	-0.622359900	-2.379671600
1	-0.523144900	-0.957712000	-3.898150600
8	2.848077400	-4.202982900	0.279862100
1	2.197611500	-4.604677700	0.881859200
1	2.300134300	-3.791604800	-0.413055300
8	4.203692100	0.208088000	-3.093132500
1	4.354744800	0.105317000	-2.131508300
1	5.011274700	0.609955800	-3.435686000
8	0.024476600	-3.243716400	3.640542700
1	0.633831600	-2.485411200	3.525225200
1	-0.833371100	-2.887458400	3.348458000

8	-3.666432900	1.359872400	-1.946206600
1	-2.823246900	0.962617300	-1.629367000
1	-3.401505100	2.222766400	-2.324025400
8	0.871635400	-2.829859800	-1.270006000
1	0.037751700	-3.186060000	-0.904280400
1	0.627294200	-2.362380100	-2.097928400
8	-2.344214400	3.611907000	-2.970802900
1	-1.766129500	3.181113700	-3.647503100
1	-2.675506900	4.418013400	-3.385353000
8	0.606298000	-5.220234400	1.853884100
1	0.446771700	-4.575475000	2.586162600
1	0.633705600	-6.088670900	2.274604000
8	-1.068427300	3.817013400	3.759040900
1	-0.575612900	4.366734000	3.101700800
1	-1.231528100	4.395137200	4.514107800
8	-3.951300900	-0.865172300	-3.592089100
1	-4.004035200	-0.031907100	-3.074225300
1	-3.815162600	-1.548593800	-2.913359400
8	0.995214700	1.841579900	-0.639754000
1	1.277696400	1.736505100	-1.577138100
1	0.999421000	0.928242800	-0.286876900
8	-1.604598900	-0.209657500	-1.090070900
1	-1.255868400	0.002854700	-0.193582500
1	-2.166668100	-1.013457500	-0.980032100
8	-1.293688200	-3.901390300	0.206789100
1	-1.491069500	-3.274702100	0.929677500
1	-0.754007100	-4.590928000	0.640833000
8	0.299414900	4.985337900	1.707633700
1	1.163318000	4.545974900	1.624626900
1	-0.189844200	4.697958400	0.912717200
8	1.624711500	1.264459700	-3.285103800
1	1.144442700	0.403525900	-3.271043100
1	2.566479700	1.003650200	-3.350716900
8	2.426205800	2.996055800	1.395113700
1	2.052835700	2.613619800	0.567894700
1	3.296049200	2.571083100	1.515224800
8	-1.091812600	0.492207100	1.464902800
1	-0.355435700	0.821882400	2.025656900
1	-1.769872800	1.197961500	1.579228300
8	1.632231500	-0.715096700	0.335717200
1	1.347922700	-1.475421400	-0.218457200
1	2.568013900	-0.550106200	0.068832100
8	4.291016100	-0.247550600	-0.319842400

1	4.585941300	0.441603600	0.316800300
1	4.685493000	-1.073878700	0.024736000
8	-0.736870700	2.239646500	-4.700876400
1	0.154772800	2.067346300	-4.347742700
1	-1.094281100	1.359563800	-4.917404600
8	4.949378400	-2.643187500	1.040221700
1	4.195915600	-3.244067500	0.822102100
1	5.736842800	-3.195761900	0.954960700
8	-4.780726200	-1.614545200	1.191788100
1	-4.905875100	-0.655722400	0.973952400
1	-5.651176700	-1.930517300	1.464446500
8	4.425089000	-0.777344500	3.223488500
1	3.453947600	-0.906319100	3.287967200
1	4.699191100	-1.488550000	2.615395800
8	1.652719200	-1.009197800	3.043218300
1	1.593991500	-0.966891300	2.058493200
1	1.314820200	-0.139563000	3.332224300
8	4.820599100	1.458856600	1.783611600
1	4.706404900	0.714040900	2.433579400
1	5.621391800	1.924932100	2.054758700
8	-1.156225900	3.585071700	-0.346898600
1	-0.482045800	2.880366900	-0.463059800
1	-1.529583000	3.717636900	-1.238172500
8	-1.784197400	-0.478991600	-5.125510300
1	-2.635351400	-0.649625900	-4.640988100
1	-1.921911900	-0.815852600	-6.019641800
8	-2.795612800	2.647124900	1.735521900
1	-2.356743400	3.129308900	1.007002500
1	-2.468768300	3.080274800	2.545631100
8	-3.256164900	-2.398699000	-1.120690400
1	-3.913151200	-2.336735700	-0.403635200
1	-2.711853800	-3.175149000	-0.888797500
8	-2.146115200	-2.025610200	2.197221500
1	-1.798693200	-1.132660000	2.003767700
1	-3.108504400	-1.949845000	2.047154200
8	-4.941587500	1.013317700	0.557249300
1	-4.621937700	1.192333800	-0.349706300
1	-4.380947700	1.583277200	1.110035500

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8	0.848480078	-3.216142418	-0.056941122
1	1.143554352	-2.279886230	-0.049201832
1	1.055267072	-3.565568061	0.832600629

8	-1.675398613	-3.154541778	-1.225608647
1	-0.824121899	-3.313183631	-0.763519348
1	-1.550087530	-3.535289382	-2.120008843
8	1.750749924	-0.601595520	-0.194408013
1	2.123129662	-0.532880178	-1.106440878
1	1.176201045	0.193821869	-0.113853501
8	1.185698252	-4.095855621	2.621027471
1	1.729196431	-3.498914335	3.191647302
1	1.484905573	-4.992973416	2.820651403
8	1.584420401	-4.446311993	-2.526006558
1	1.419693442	-4.092805684	-1.630717371
1	0.694664075	-4.535136701	-2.919090154
8	-1.387600590	-2.876525583	2.719509591
1	-0.616473177	-3.474174244	2.756923324
1	-1.046832644	-2.082396885	2.249465285
8	-1.476334845	-0.451092045	-1.040004071
1	-1.614498041	-1.418657566	-1.181910773
1	-1.123650465	-0.395411069	-0.122568887
8	-0.854551117	-0.409673601	1.654170116
1	-0.138708618	0.107955263	2.077098465
1	-1.668040572	-0.037746827	2.063247799
8	-0.955200893	-4.099092353	-3.743429673
1	-0.666260718	-3.309711442	-4.274055864
1	-1.502858874	-4.632956711	-4.333324243
8	3.244936817	-0.300553117	2.013942911
1	2.812222769	-0.501475912	1.146029166
1	3.910325364	0.372151282	1.783248357
8	2.561979644	-0.247057890	-2.763183591
1	2.748732037	-1.063444496	-3.272487427
1	1.676369343	0.043592668	-3.070383419
8	2.536632720	-2.227391424	4.066669612
1	2.936448887	-1.615343860	3.422677211
1	1.895570973	-1.681608720	4.563944564
8	-3.642388468	-2.882619924	0.883351018
1	-3.134289643	-3.072737143	0.074942006
1	-2.999785260	-3.060377714	1.592852606
8	2.713783363	-2.646737022	-4.166852975
1	2.404882984	-3.360829002	-3.547804167
1	3.491852920	-2.999111121	-4.616076101
8	-0.100958860	0.347570670	-3.306810639
1	-0.581025171	0.122153761	-2.481191310
1	-0.443972407	1.220415739	-3.582276827
8	0.480753036	1.844760622	0.028616843

1	-0.411840736	2.004041909	0.399448615
1	1.066921432	2.343355670	0.640320747
8	0.084439243	-1.956740869	-4.982335682
1	1.042189208	-2.128268059	-4.894443524
1	-0.059320240	-1.126443276	-4.489353348
8	1.139644135	1.008026203	3.117045940
1	1.938839306	0.522103549	2.791898177
1	0.989806333	0.645476805	4.014187239
8	-1.885773137	-1.155794080	4.846342428
1	-1.805539441	-1.881641905	4.188231528
1	-2.373861197	-0.462870489	4.367850648
8	0.645926573	-0.542046312	5.374704360
1	-0.317360161	-0.768278885	5.235754543
1	0.741863942	-0.389835301	6.324070624
8	-3.102672159	0.700768012	2.859751211
1	-3.851800772	0.382946381	2.317654054
1	-2.847394625	1.552529065	2.448190906
8	3.833542026	2.147649976	-1.745164003
1	3.597020228	1.298283219	-2.155924263
1	3.087643776	2.724002361	-1.987041923
8	-3.504415013	1.295496779	-0.847244240
1	-2.835468032	0.590915700	-1.041069932
1	-4.218400662	0.810055035	-0.397059821
8	-4.922169646	-0.459545513	1.012445163
1	-4.507190465	-1.353000925	0.946940473
1	-5.853030448	-0.629323589	1.204792163
8	4.492577770	2.105345657	0.917327504
1	4.308357715	2.116158135	-0.051728300
1	5.360797661	2.519913079	1.011893040
8	-2.071288072	2.566320246	1.074390569
1	-2.641013533	2.171817974	0.366995610
1	-2.076907998	3.525426282	0.876526633
8	2.065078906	3.280343875	1.808494175
1	1.745142081	2.676330587	2.510656061
1	2.975877594	2.977442706	1.622742988
8	1.243533295	3.428201688	-2.072458917
1	0.870194530	2.760576545	-1.454514926
1	0.633833512	3.408112612	-2.834241895
8	-0.901507632	3.005918175	-3.899958402
1	-1.685169354	3.329441437	-3.390295727
1	-1.042574102	3.296076112	-4.809654111
8	-2.937900300	3.766344231	-2.261614926
1	-3.284743026	2.952311282	-1.855389022

1	-2.573324646	4.281724792	-1.515051661
8	0.814945629	5.264391806	-0.028336818
1	1.247610751	4.783670968	0.698524421
1	1.058686656	4.747097534	-0.828182742
8	-1.839485287	5.120353091	-0.006335758
1	-0.846266548	5.233358809	-0.000029320
1	-2.199717137	5.983201784	0.235007622

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8	-3.326253449	0.663173649	1.768114551
1	-3.277150906	0.656319021	2.741598053
1	-2.547611107	1.185407613	1.482537571
8	-2.678973818	0.567902381	4.498764283
1	-1.715482306	0.457729073	4.601532882
1	-3.063055376	0.308001035	5.340556517
8	-1.081427861	1.902343462	0.714037153
1	-1.267488716	2.229261893	-0.194823046
1	-0.518648235	2.602546851	1.117161975
8	-2.786701305	-1.866262444	0.787239237
1	-3.074655209	-1.035805325	1.217160590
1	-3.573796618	-2.188227147	0.307116665
8	-4.989884400	0.557071913	-0.568862779
1	-4.537733714	0.641818769	0.289989029
1	-4.969292894	-0.398148838	-0.770107810
8	0.559492592	-0.031899491	1.788853745
1	-0.002304947	0.581267011	1.264213509
1	0.370481101	0.204648503	2.724891670
8	-1.176752569	-0.881952401	-1.320712365
1	-1.715535200	-1.160093361	-0.550383436
1	-0.932559658	-1.740997901	-1.743256396
8	-4.867064685	-2.275118715	-0.997145792
1	-4.347727201	-2.532199674	-1.809262239
1	-5.640054292	-2.850621073	-0.989097063
8	0.135217973	0.543179637	4.481092403
1	0.561231683	1.414319962	4.602318264
1	0.747571513	-0.099252624	4.886575826
8	-0.196745968	-2.638436755	1.465397956
1	-1.166420955	-2.614277009	1.372404967
1	0.042558645	-1.688304090	1.539523699
8	-1.550563720	3.024433434	-1.760955562
1	-2.441516918	2.839777469	-2.116231192
1	-0.902304388	2.769211093	-2.456920215
8	-4.085861352	2.102933208	-2.555118287

1	-4.472345082	1.575216077	-1.804997323
1	-4.817532583	2.619021823	-2.913745409
8	0.851856206	3.615451013	1.634699779
1	1.155633832	3.480367769	2.553485368
1	1.544496312	3.207108730	1.061039737
8	-2.600441173	-0.099398995	-3.532752651
1	-2.143377691	-0.188890721	-2.665412330
1	-3.181073349	0.676896993	-3.425280058
8	1.187674063	0.474357958	-1.468784409
1	0.316043710	0.062714068	-1.273880046
1	1.755213821	-0.305564573	-1.685899698
8	-3.404032182	-2.776772704	-3.153950737
1	-3.219962416	-1.864672034	-3.459799666
1	-2.516807879	-3.137350748	-2.978144840
8	1.698546048	2.867576498	4.276196282
1	2.474359470	2.246182813	4.232246850
1	1.937918739	3.534458688	4.930562272
8	0.056224718	5.122319704	-0.671663992
1	-0.671124027	4.550910405	-0.981122543
1	0.234976369	4.822138929	0.237555813
8	-0.567833633	-3.238867283	-2.613525557
1	0.020646280	-3.713233596	-1.996985345
1	0.019324485	-2.979433043	-3.353477956
8	1.895649206	-3.266338968	3.266201450
1	1.058887253	-3.214887524	2.769272229
1	2.545398313	-3.570183144	2.606740587
8	2.498777316	2.506158509	-0.225269782
1	1.968060952	1.805527402	-0.669063525
1	2.651674698	3.174569101	-0.922086804
8	3.284916503	0.352534998	1.421531751
1	2.316335625	0.182864058	1.473796408
1	3.334060264	1.152150081	0.865466534
8	2.152648730	-1.318518341	5.154687778
1	2.113682447	-2.039294616	4.483621838
1	2.311527868	-1.770069429	5.993178215
8	1.262842623	-3.789521628	-0.547020631
1	0.727808380	-3.371021031	0.163021002
1	2.015392710	-4.179244293	-0.060567167
8	0.578585915	2.354293334	-3.355795199
1	0.919047508	1.679460921	-2.727704440
1	1.174626285	3.117828283	-3.226909970
8	3.577991063	0.961623238	4.099849416
1	3.609933133	0.727967803	3.146308865

1	3.228766792	0.154590981	4.520752618
8	-0.205396784	0.109759698	-4.996497476
1	-1.101650115	0.074268597	-4.605165312
1	0.162233927	0.938488735	-4.642496587
8	2.531130878	-1.814241994	-2.086469880
1	2.069040583	-2.516961142	-1.579261437
1	2.286236803	-1.973321056	-3.019177668
8	2.135475362	4.427884082	-2.243460875
1	1.419223285	4.839223379	-1.696465851
1	2.651371748	5.161121218	-2.602968409
8	4.395904133	-1.856639713	0.061942652
1	4.069357451	-1.082926313	0.566199631
1	3.973017861	-1.758431845	-0.810770113
8	1.167951998	-2.119044723	-4.509587593
1	0.685207506	-1.272224340	-4.727397063
1	1.405031231	-2.501565424	-5.362573020
8	3.498411012	-4.136607837	1.079506599
1	3.935824125	-3.313035417	0.719325804
1	4.194975822	-4.799977391	1.148669128

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8	1.518998097	3.684914304	1.322676204
1	0.789453241	4.293586598	1.557066584
1	1.489192676	3.646298445	0.342737404
8	3.024615767	-0.047945013	3.890484615
1	3.236750418	0.827166019	3.479298329
1	3.508214812	-0.059561404	4.726138463
8	-4.296183400	0.788203428	-2.184044874
1	-3.978065883	1.689673726	-2.005593075
1	-4.733599022	0.484525151	-1.367279391
8	-4.474666973	-2.907326973	0.471008613
1	-4.942408897	-2.053720762	0.383090184
1	-3.899017219	-2.940424875	-0.313244231
8	-3.117865680	-0.938823674	-3.912761592
1	-3.747561804	-1.061804476	-4.634248169
1	-3.527117984	-0.253642895	-3.330727196
8	-2.617484461	-0.869564291	4.138116120
1	-1.654084038	-0.727492879	4.140490780
1	-2.725224109	-1.784941071	3.823991328
8	-2.653415584	3.061750100	-1.573415040
1	-2.177194330	3.927440975	-1.612057081
1	-1.962555954	2.423484075	-1.853306102
8	-0.946698232	5.192903870	-1.341938099

1	-0.932910228	5.365720256	-0.381638871
1	-0.102089574	4.732379895	-1.499625851
8	5.408809922	-1.431441572	-0.151039240
1	4.961679842	-1.833144955	-0.944679619
1	6.292359708	-1.818510206	-0.124454529
8	3.634004910	2.269450409	-2.380839402
1	4.194692986	2.639297931	-3.074400410
1	3.314818295	1.406343569	-2.722886181
8	-0.263962544	-0.712420262	-3.809148612
1	-1.182089348	-0.802883943	-4.121483388
1	-0.108655577	-1.503648346	-3.246976495
8	5.013178227	1.461920986	0.146547048
1	5.183513963	0.514928729	0.005229768
1	4.584432687	1.758391451	-0.672862262
8	-2.579534359	-2.541932870	-1.673454044
1	-2.814954816	-2.163905938	-2.543698865
1	-1.623516378	-2.758393954	-1.742638417
8	-2.951147830	-3.323869017	2.632698235
1	-3.562180712	-3.144906959	1.866645821
1	-3.208284141	-4.196272147	2.956824697
8	2.177995339	-4.488245140	-1.541269833
1	2.183412669	-5.428174519	-1.757744469
1	2.090240063	-4.431904738	-0.552445403
8	-3.559325778	0.458440394	1.909000785
1	-2.922941831	0.043814107	1.277186228
1	-3.325308454	0.050748885	2.775987477
8	3.274412626	-1.600894347	1.517042628
1	3.354418397	-1.150826956	2.377862329
1	4.156306379	-1.550553770	1.086608850
8	0.188191703	-0.481374710	3.442485145
1	1.093509476	-0.408420194	3.793710330
1	0.155087690	0.218659334	2.751339191
8	-0.471355853	-2.530920826	1.679319023
1	-0.177356820	-1.933036495	2.399270809
1	-1.295942672	-2.938487762	2.025218558
8	2.422153304	-0.164522913	-2.823735026
1	1.665037409	-0.183412485	-3.433239196
1	2.015330725	-0.198421614	-1.925392461
8	1.858217437	-4.023427623	1.067232178
1	0.980806584	-3.637623964	1.267518792
1	2.469593792	-3.309720315	1.329856917
8	1.187891666	3.270706796	-1.399192961
1	0.622087696	2.477575575	-1.508951505

1	2.041183075	3.041467287	-1.818300667
8	0.176290151	-2.565300216	-1.824950289
1	0.556146193	-1.945498706	-1.160566649
1	0.800055433	-3.319815241	-1.843557131
8	0.148279456	1.287639739	1.326033014
1	0.706842802	2.093390839	1.430037488
1	-0.740443575	1.676185547	1.151606609
8	-5.497659689	-0.259832044	0.227002086
1	-4.958100458	0.072232801	0.989453983
1	-6.411035809	-0.004757001	0.410526192
8	-1.795942442	-0.588639817	0.085458860
1	-2.229566520	-1.199518410	-0.556564247
1	-1.198285582	-1.196742973	0.575337792
8	1.418185098	-0.574711346	-0.290562733
1	2.085158280	-0.888590405	0.362095513
1	0.935855998	0.144761085	0.181176474
8	-2.221204546	2.720640323	1.060788000
1	-2.868617603	2.124716820	1.489333744
1	-2.508362480	2.819785558	0.113868255
8	-0.922245091	5.042537255	1.549797455
1	-1.256886937	5.646166528	2.224407604
1	-1.519486165	4.257143781	1.561145722
8	3.669846164	2.233061972	2.567735931
1	4.141394876	1.970028749	1.754238592
1	2.965707187	2.821685969	2.242697892
8	4.050039124	-2.371149942	-2.246562500
1	3.480489600	-1.658735960	-2.604821291
1	3.462009831	-3.135658140	-2.123628618
8	-0.660009809	1.178770500	-1.801731060
1	-0.529685153	0.576530880	-2.566436089
1	-0.989110435	0.590674615	-1.089442475

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8	0.872033555	3.755254190	1.365702357
1	0.034615805	4.249010594	1.525106761
1	0.951346216	3.772530703	0.392607230
8	2.848993470	0.332760587	4.068719353
1	2.972406856	1.220886416	3.647840476
1	3.301535716	0.384808629	4.918052267
8	-2.780852852	-1.424951837	-3.997021949
1	-3.332485151	-0.781996997	-3.474664244
1	-3.348971541	-1.695542548	-4.728650819
8	-4.321276798	-0.718412301	0.183803683

1	-4.624362395	-0.291790109	1.006912370
1	-3.337683639	-0.651358201	0.225036988
8	-4.324278546	0.211139315	-2.525404133
1	-4.513716381	-0.103475314	-1.621254540
1	-4.063707494	1.139759625	-2.396738301
8	-2.668785440	-1.033284427	3.909321544
1	-1.726544583	-0.792620866	3.957150793
1	-2.674681992	-1.923846056	3.510698127
8	-2.966664052	2.565844116	-1.704482753
1	-2.678863116	3.497066432	-1.784399162
1	-2.154534967	2.056179322	-1.926594545
8	-1.692118117	4.768268069	1.393576896
1	-2.155008999	3.906874418	1.381823669
1	-1.764784840	5.065969015	0.469943278
8	2.595525428	0.140402776	-2.888880338
1	1.899563577	0.022300443	-3.555809332
1	2.112043391	0.125570643	-2.040489116
8	3.288353964	2.990645361	-2.368373314
1	3.709256867	2.782632034	-1.514190228
1	3.235093664	2.114667848	-2.786930237
8	-0.003852703	-0.755547898	-3.899335451
1	-0.899550732	-0.986027335	-4.210728650
1	0.271503866	-1.514844745	-3.346172869
8	5.513108638	-0.660915745	0.143858208
1	5.205761481	-1.103451949	-0.697845652
1	6.472490529	-0.763512788	0.166076206
8	-1.998977015	-3.037120881	-1.832979669
1	-2.276784515	-2.641015760	-2.683183658
1	-1.020144840	-3.085019243	-1.883124891
8	-2.558332344	-3.579621062	2.547179541
1	-2.738069369	-4.415585026	2.996045414
1	-3.130799924	-3.588753758	1.728879487
8	2.969628133	-4.118636431	-1.398660778
1	3.146910503	-5.030756547	-1.658931794
1	2.767233269	-4.141087725	-0.429344482
8	-4.439527581	0.631457265	2.664926978
1	-3.828475852	0.070203052	3.197737315
1	-5.111675848	0.947350743	3.282035874
8	3.368326611	-1.253621915	1.757097509
1	3.354868622	-0.799514823	2.619852285
1	4.251749211	-1.083671745	1.366819461
8	0.138475002	-0.422818237	3.506748551
1	0.044871450	0.241798233	2.787123132

1	1.004401137	-0.215970817	3.905245010
8	-0.185537338	-2.495346322	1.702158550
1	0.015332961	-1.899692943	2.454431410
1	-0.951459348	-3.026040694	2.018518626
8	3.878362215	1.644465730	0.153562220
1	4.600627163	0.986123421	0.133624642
1	3.088592219	1.105566915	-0.048459342
8	2.303849308	-3.826398904	1.195378189
1	1.387076279	-3.503658390	1.302749918
1	2.820663046	-3.057715562	1.503359654
8	0.728454311	3.415447609	-1.449623094
1	0.331461197	2.532615884	-1.584149639
1	1.621137403	3.360828207	-1.865875306
8	0.730200296	-2.508529858	-1.854909389
1	0.961184411	-1.815820187	-1.203749904
1	1.478966425	-3.138038317	-1.822608732
8	-0.130923113	1.204381808	1.308891985
1	0.247795108	2.113516123	1.405706528
1	-1.081743897	1.382880785	1.116149619
8	-3.989210729	-3.477666745	0.308252264
1	-3.397897484	-3.572184283	-0.458566264
1	-4.281335628	-2.539872160	0.249534716
8	-1.627570751	-0.929352885	-0.125654302
1	-1.805870080	-1.671996019	-0.752240915
1	-1.061247806	-1.359976352	0.554282137
8	1.635481593	-0.249751187	-0.197395464
1	2.159524277	-0.655696018	0.532778398
1	0.917134045	0.251563207	0.262254276
8	-2.698920457	2.122262984	0.985326487
1	-3.008426215	2.212052285	0.054477968
1	-3.420260453	1.728918483	1.509835576
8	-1.518873087	4.998355946	-1.552304962
1	-1.504827713	5.765913690	-2.135469933
1	-0.629360025	4.584442936	-1.638646476
8	3.210568141	2.633409351	2.682932586
1	3.541834541	2.322130116	1.813617565
1	2.437565741	3.170475114	2.439394056
8	4.472017841	-1.743735661	-2.021301223
1	4.014985400	-2.597181787	-1.923009344
1	3.839514945	-1.147880542	-2.477728226
8	-0.714408613	1.022414042	-1.891078357
1	-0.479030760	0.464630884	-2.664791135
1	-0.965513767	0.372209356	-1.197508855

Figure S1: MTA-based convoluted spectra (full-width at half-maximum of 10 cm^{-1}) of W32-T7 isomer at MP2/aug-cc-pvDZ level of theory.

Figure S2: MTA-based convoluted spectra (full-width at half-maximum of 10 cm^{-1}) of W32-TIP4P/2005 isomer at MP2/aug-cc-pvDZ level of theory.

Figure S3: MTA-based convoluted spectra (full-width at half-maximum of 10 cm^{-1}) of W32-G1 isomer at MP2/aug-cc-pvDZ level of theory.

Figure S4: MTA-based convoluted spectra (full-width at half-maximum of 10 cm^{-1}) of W32-TIP4P isomer at MP2/aug-cc-pvDZ level of theory.

Figure S5: MTA-based convoluted spectra (full-width at half-maximum of 10 cm^{-1}) of W32-G2 isomer at MP2/aug-cc-pvDZ level of theory.

Figure S6: MTA-based convoluted spectra (full-width at half-maximum of 10 cm^{-1}) of W32-TIP4P-Ew isomer at MP2/aug-cc-pvDZ level of theory.