

Supplementary Information

Thermodynamics of Oligomer Formation: Implications for Secondary Organic Aerosol Formation and Reactivity

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Figure S1. Comparison of the gas phase (a and c) and water solvated (b and d) geometries for the *cis*-pinic acid non-covalent dimerization pathway at 298 K. Carbon atoms are gray, oxygen atoms are red and hydrogen atoms are white. Hydrogen bonds indicated with dashed lines.

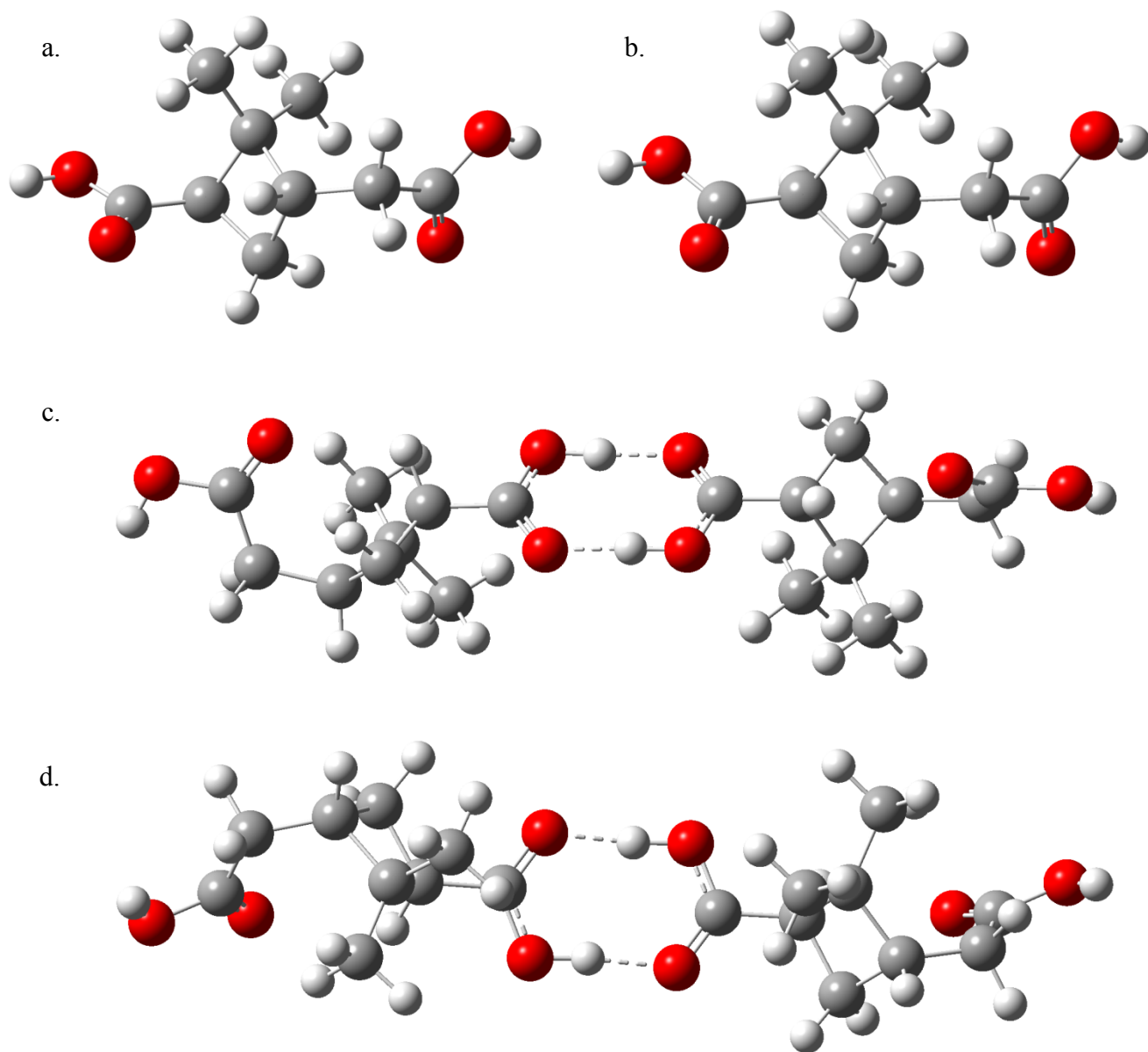


Figure S2. Comparison of the gas phase (a and c) and water solvated (b and d) geometries for the peroxyhemiacetal covalent dimerization pathway at 298 K. Carbon atoms are gray, oxygen atoms are red and hydrogen atoms are white.

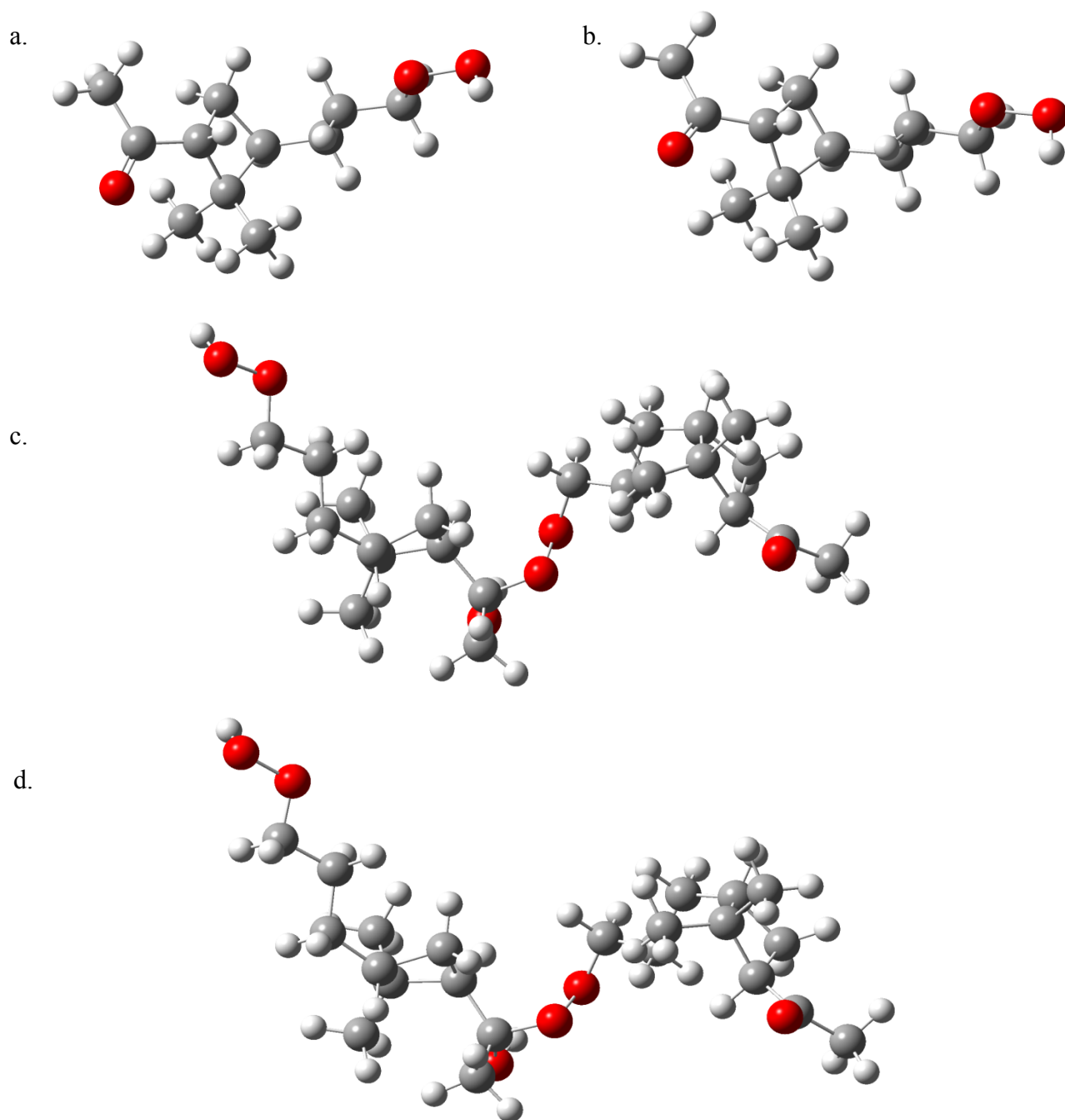


Table S1. Benchmark information for gas phase dimerization free energies calculated using PW91 with the 6-311++G(2d,2p) and 6-311++G(3df,3pd) basis sets at 298 K. Calculated as single point energies using the appropriate geometry and thermal correction to the free energy from PW91/6-31+G(d,p) basis set. Values are in atomic units (hartrees) except where noted.

Basis Set	6-311++G(2d,2p)			6-311++G(3df,3pd)		
Molecule	E _{SCF}	G _{corr}	ΔG (kJ/mol)	E _{SCF}	G _{corr}	ΔG (kJ/mol)
cis-pinic acid	-652.2864481	0.178181	-24.63857417	-652.3099267	0.178181	-26.5506523
c-PA dimer	-1304.585471	0.359552		-1304.633156	0.359552	
terpenylic acid	-612.9994663	0.153695	-29.10555786	-613.0220257	0.153695	-30.0438748
TA dimer	-1226.029609	0.326981		-1226.075086	0.326981	

Table S2. Benchmark information for condensed phase (water based) dimerization free energies calculated using PW91 with the 6-311++G(2d,2p) and 6-311++G(3df,3pd) basis sets at 298 K. Calculated as single point energies using the appropriate geometry and thermal correction to the free energy from PW91/6-31+G(d,p) basis set and using the guidelines for solvent modeling given in the Computational Methods section in the manuscript. Values are in hartrees except where noted.

Basis Set	6-311++G(2d,2p)			6-311++G(3df,3pd)		
Molecule	E _{SCF}	G _{corr}	ΔG (kJ/mol)	E _{SCF}	G _{corr}	ΔG (kJ/mol)
cis-pinic acid	-652.2864481	0.177234	-29.21110434	-652.3099267	0.177234	-30.30822202
c-PA dimer	-1304.585471	0.376003		-1304.633156	0.376003	
terpenylic acid	-612.9994663	0.15242	-4.288797635	-613.0220257	0.15242	-5.392883397
TA dimer	-1226.029609	0.326693		-1226.075086	0.326693	

Table S3. Extended thermochemical information for all gas phase monomers and dimers studied at 298 K. All data given in atomic units (hartrees) and calculated at 1 atm standard pressure. E_0 is the total electronic energy plus the calculated zero-point energy.

	$E_{\text{electronic}}$	E_0	H	G
Monomers and Dimers				
Aldehyde/Ester, Monomer 1	-613.9886324	-613.774962	-613.760717	-613.81498
Norpinic Acid	-612.8163022	-612.625122	-612.611481	-612.664714
Water	-76.40614442	-76.385374	-76.381594	-76.403047
<i>cis</i> -Pinic Acid	-652.1170908	-651.897756	-651.882923	-651.939023
Pinonaldehyde	-540.9333194	-540.69855	-540.683672	-540.739374
<i>cis</i> -Pinonic Acid	-616.1829323	-615.942516	-615.926797	-615.985277
Hemi-acetal, Monomer 1	-691.3748758	-691.129607	-691.113146	-691.172996
Hydroperoxide Monomer	-616.5539273	-616.265256	-616.246954	-616.311105
2,2-dimethyl-3-formyl-cyclobutyl-methanoic acid	-614.001715	-613.788042	-613.773866	-613.827351
Terpenylic Acid	-612.8391131	-612.646997	-612.633867	-612.685447
Anhydride Dimer	-1150.378773	-1149.998549	-1149.97223	-1150.05702
<i>cis</i> -Pinic Acid Dimer	-1304.246025	-1303.807751	-1303.777582	-1303.888326
Ester Dimer	-1150.388493	-1150.007643	-1149.981583	-1150.066283
Aldol Addition Dimer	-1157.124428	-1156.644819	-1156.614859	-1156.705867
Hemi-acetal Dimer	-1232.320842	-1232.319765	-1231.804217	-1231.898657
Peroxyhemiacetal Dimer	-1233.065018	-1232.539042	-1232.503656	-1232.627733
Di(α -hydroxy) Ether Dimer	-1230.180364	-1229.721777	-1229.692819	-1229.781454
Terpenylic Acid Dimer	-1225.710232	-1225.325059	-1225.298599	-1225.383575
TA-cPA non-covalent Dimer (alkyl carboxylate)	-1264.987068	-1264.574749	-1264.546601	-1264.636033
TA-cPA non-covalent Dimer (carboxylate)	-1264.986692	-1264.574331	-1264.5462	-1264.63554

Table S4. Extended thermochemical information for all gas phase monomers and dimers studied at 373 K. All data given in atomic units (hartrees) and calculated at 1 atm standard pressure.

	E_{electronic}	E₀	H	G
Monomer and Dimers				
Aldehyde/Ester, Monomer 1	-613.988632	-613.774962	-613.753931	-613.829364
Norpinic Acid	-612.816302	-612.625122	-612.604996	-612.678807
Water	-76.406144	-76.385374	-76.380633	-76.408544
<i>cis</i> -Pinic Acid	-652.1170907	-651.897756	-651.875806	-651.953905
Pinonaldehyde	-540.9333193	-540.698518	-540.676636	-540.754148
<i>cis</i> -Pinonic Acid	-616.1829323	-615.942516	-615.919322	-616.000797
Hemi-acetal, Monomer 1	-691.374876	-691.129607	-691.105248	-691.188907
Hydroperoxide Monomer	-617.256129	-616.995445	-616.970569	-617.055599
Terpenylic Acid	-612.8391131	-612.646997	-612.627515	-612.69911
Anhydride Dimer	-1150.378773	-1149.998549	-1149.95954	-1150.079731
<i>cis</i> -Pinic Acid Dimer	-1304.246025	-1303.807751	-1303.763095	-1303.897857
Ester Dimer	-1150.379399	-1149.998549	-1149.95954	-1150.079731
Aldol Addition Dimer	-1157.138285	-1156.658676	-1156.61372	-1156.745885
Hemi-acetal Dimer	-1232.320842	-1231.835882	-1231.790319	-1231.925249
Peroxyhemiacetal Dimer		-1233.999574	-1233.950727	-1234.091316
Terpenylic Acid Dimer	-1225.71023	-1225.325059	-1225.285752	-1225.40635
TA-cPA non-covalent Dimer (alkyl carboxylate)	-1264.987068	-1264.574759	-1264.532996	-1264.660087
TA-cPA non-covalent Dimer (carboxylate)	-1264.986692	-1264.574331	-1264.532592	-1264.659496

Table S5. Extended thermochemical information for all monomers and dimers studied in the water solvent continuum at 298 K. All data given in atomic units (hartrees) and calculated at 1 M standard concentration.

	E_{electronic}	E₀	H	G
Monomers and Dimers				
Aldehyde/Ester, Monomer 1	-614.008066	-613.794961	-613.780848	-613.834314
Norpinic Acid	-612.841869	-612.651522	-612.638034	-612.690262
Water	-76.419787	-76.399267	-76.395487	-76.416952
<i>cis</i> -Pinic Acid	-652.136101	-651.917986	-651.903213	-651.958867
Pinonaldehyde	-540.947935	-540.71382	-540.698992	-540.75408
<i>cis</i> -Pinonic Acid	-616.200257	-615.960121	-615.944816	-616.001221
Hemi-acetal, Monomer 1	-691.402217	-691.157485	-691.141122	-691.200122
Hydroperoxide Monomer	-656.572585	-656.283898	-656.266071	-656.328372
2,2-dimethyl-3-formyl-cyclobutyl-methanoic acid	-614.023523	-613.811463	-613.797016	-613.8511
Terpenylic Acid	-612.8622	-612.671196	-612.658	-612.70978
Anhydride Dimer	-1150.40658	-1150.027329	-1150.001246	-1150.083976
<i>cis</i> -Pinic Acid Dimer	-1304.284761	-1303.847501	-1303.817789	-1303.908758
Ester Dimer	-1150.424067	-1150.044457	-1150.018682	-1150.100762
Aldol Addition Dimer	-1157.156374	-1156.693331	-1156.663888	-1156.752049
Hemi-acetal Dimer	-1232.360469	-1231.875708	-1231.845495	-1231.937455
Peroxyhemiacetal Dimer	-1313.151544	-1312.571296	-1312.536062	-1312.63972
Di(α -hydroxy) Ether Dimer	-1230.212123	-1229.75576	-1229.726795	-1229.814345
Terpenylic Acid Dimer	-1225.744199	-1225.360902	-1225.334572	-1225.417506
TA-cPA non-covalent Dimer (alkyl carboxylate)	-1265.01657	-1264.607566	-1264.57919	-1264.668765
TA-cPA non-covalent Dimer (carboxylate)	-1265.016683	-1264.606983	-1264.578894	-1264.667498

Table S6. Extended thermochemical information for all monomers and dimers studied in the water solvent continuum at 373 K. All data given in atomic units (hartrees) and calculated at 1 M standard concentration.

	E_{electronic}	E₀	H	G
Monomers and Dimers				
<i>cis</i> -Pinic Acid	-652.1361011	-651.917986	-651.896055	-651.973642
Pinonaldehyde	-540.9479353	-540.71382	-540.691939	-540.769236
<i>cis</i> -Pinonic Acid	-616.2002563	-615.960121	-615.937355	-616.016218
Hydroperoxide Monomer	-657.2744961	-657.013693	-656.989347	-657.071996
Terpenylic Acid	-612.8622006	-612.671196	-612.651613	-612.723497
<i>cis</i> -Pinic Acid Dimer	-1304.284761	-1303.847501	-1303.803283	-1303.933224
Aldol Addition Dimer	-1157.170235	-1156.693308	-1156.649135	-1156.775843
Peroxyhemiacetal Dimer	-1314.554902	-1314.02897	-1313.980846	-1314.117865
Terpenylic Acid Dimer	-1225.744198	-1225.360902	-1225.321676	-1225.439775
TA-cPA non-covalent Dimer (alkyl carboxylate)	-1265.01657	-1264.607565	-1264.565452	-1264.692795
TA-cPA non-covalent Dimer (carboxylate)	-1265.016683	-1264.606983	-1264.578894	-1264.667498

Table S7. Extended thermochemical information for all monomers and dimers studied in the methanol solvent continuum at 298 K. All data given in atomic units (hartrees) and calculated at 1 M standard concentration.

	E_{electronic}	E₀	H	G
Monomers and Dimers				
<i>cis</i> -Pinic Acid	-652.1404442	-651.922103	-651.907344	-651.963116
Pinonaldehyde	-540.9539212	-540.719476	-540.704825	-540.759436
<i>cis</i> -Pinonic Acid	-616.205946	-615.965748	-615.950406	-616.00693
Hydroperoxide Monomer	-656.5812004	-656.292482	-656.274668	-656.336694
Terpenylic Acid	-612.8650724	-612.673862	-612.660693	-612.712241
<i>cis</i> -Pinic Acid Dimer	-1304.29148	-1303.853688	-1303.824107	-1303.914686
Aldol Addition Dimer	-1157.16564	-1156.703411	-1156.673819	-1156.764175
Peroxyhemiacetal Dimer	-1313.167383	-1312.587192	-1312.550221	-1312.654901
Terpenylic Acid Dimer	-1225.749083	-1225.365376	-1225.337193	-1225.440668
TA-cPA non-covalent Dimer (alkyl carboxylate)	-1265.023118	-1264.613931	-1264.585562	-1264.675609
TA-cPA non-covalent Dimer (carboxylate)	-1265.02332	-1264.612867	-1264.584872	-1264.672615

Table S8. Extended thermochemical information for all monomers and dimers studied in the methanol solvent continuum at 373 K. All data given in atomic units (hartrees) and calculated at 1 M standard concentration.

	E_{electronic}	E₀	H	G
Monomers and Dimers				
<i>cis</i> -Pinic Acid	-652.1404442	-651.922103	-651.9002	-651.977919
Pinonaldehyde	-540.9539212	-540.719476	-540.697789	-540.773935
<i>cis</i> -Pinonic Acid	-616.205946	-615.965748	-615.942954	-616.021956
Hydroperoxide Monomer	-657.2821483	-657.021265	-656.996991	-657.079177
Terpenylic Acid	-612.8650724	-612.673862	-612.654319	-612.725897
<i>cis</i> -Pinic Acid Dimer	-1304.291483	-1303.853688	-813.809641	-1303.939049
Aldol Addition Dimer	-1157.179497	-1156.703411	-1156.659066	-1156.788513
Peroxyhemiacetal Dimer	-1314.56882	-1314.043616	-1313.995238	-1314.132915
Terpenylic Acid Dimer	-1225.749083	-1225.365376	-1225.322667	-1225.490123
TA-cPA non-covalent Dimer (alkyl carboxylate)	-1265.023118	-1264.613931	-1264.571844	-1264.699755
TA-cPA non-covalent Dimer (carboxylate)	-1265.02332	-1264.612867	-1264.571214	-1264.696175

Table S9. Ratios of dimer fractions $[(f_{\text{dimer},373})/(f_{\text{dimer},298})]$ of remaining favorable condensed phase dimers in water and methanol derived using the predicted standard state $\Delta G_a^\circ(aq \text{ or } solv)$ for each pathway.

	cPA-TA non-covalent dimer (alkyl carboxylate)	cPA-TA non-covalent dimer (alkyl carboxylate)	cPA-TA non-covalent dimer (carboxylate)	cPA-TA non-covalent dimer (carboxylate)	Peroxy-hemiacetal	Peroxy-hemiacetal
Mass Fraction of Monomer in total SOA mass	Water	Methanol	Water	Methanol	Water	Methanol
0.0001	5.09E-01	2.94E-01	1.86E+02	1.53E-02	1.20E-02	5.17E-02
0.0005	2.02E-01	1.16E-01	7.43E+01	6.18E-03	2.28E-03	1.68E-03
0.001	5.07E-01	2.88E-01	1.86E+02	1.57E-02	4.45E-04	2.21E-04
0.005	2.02E-01	1.15E-01	7.40E+01	6.95E-03	8.75E-07	2.59E-06
0.0075	3.37E-01	1.92E-01	1.23E+02	1.23E-02	2.81E-06	7.51E-06
0.01	5.07E-01	2.88E-01	1.85E+02	1.95E-02	4.16E-06	2.38E-06
0.025	3.01E-01	1.71E-01	1.96E+02	1.50E-02	2.28E-06	1.69E-06
0.05	1.96E-01	1.12E-01	7.10E+01	1.34E-02	1.29E-07	2.09E-07
0.075	3.29E-01	1.87E-01	1.16E+02	2.81E-02	1.23E-06	3.49E-07
0.1	5.07E-01	2.88E-01	1.72E+02	5.12E-02	7.05E-07	3.46E-07

Cartesian coordinates for optimized gas phase monomers and dimers studied in the article

Aldehyde/Ester Monomer 1 – Gas Phase @ 298 K

O	-3.2129340	0.5744150	-0.9006070
C	-2.9834380	-0.7626400	-0.4788900
O	-2.0000960	-0.8920520	0.5283130
C	-0.6519270	-0.7184540	0.0938410
C	0.3947810	-1.3491830	1.0248130
C	1.3153800	-0.1169280	0.8031150
C	0.0465990	0.6821350	0.2448690
C	0.2072570	1.4971760	-1.0364820
C	-0.5547580	1.5330920	1.3671370
C	2.3874020	-0.3357860	-0.2277400
O	2.3821210	-1.1837510	-1.1126970
O	3.4041130	0.5725550	-0.1023890
H	-3.6291050	1.0532820	-0.1603490
H	-3.8936370	-1.2110060	-0.0468400
H	-2.6812110	-1.3008790	-1.3945070
H	-0.5463610	-1.0843840	-0.9444120
H	0.7973380	-2.3277170	0.7303530
H	0.0278610	-1.3915790	2.0603000
H	1.7603730	0.3400860	1.6986120
H	0.6640570	0.9032840	-1.8438620
H	-0.7841940	1.8280340	-1.3851650
H	0.8325920	2.3894250	-0.8688590
H	0.1167270	2.3743450	1.6037400
H	-1.5240560	1.9493000	1.0518790
H	-0.7229190	0.9536030	2.2876530
H	4.0291250	0.3783930	-0.8334750

Aldehyde/Ester Monomer 1 – Gas Phase @ 373 K

O	-3.2129340	0.5744150	-0.9006070
C	-2.9834380	-0.7626400	-0.4788900
O	-2.0000960	-0.8920520	0.5283130
C	-0.6519270	-0.7184540	0.0938410
C	0.3947810	-1.3491830	1.0248130
C	1.3153800	-0.1169280	0.8031150
C	0.0465990	0.6821350	0.2448690
C	0.2072570	1.4971760	-1.0364820
C	-0.5547580	1.5330920	1.3671370
C	2.3874020	-0.3357860	-0.2277400
O	2.3821210	-1.1837510	-1.1126970
O	3.4041130	0.5725550	-0.1023890
H	-3.6291050	1.0532820	-0.1603490

H	-3.8936370	-1.2110060	-0.0468400
H	-2.6812110	-1.3008790	-1.3945070
H	-0.5463610	-1.0843840	-0.9444120
H	0.7973380	-2.3277170	0.7303530
H	0.0278610	-1.3915790	2.0603000
H	1.7603730	0.3400860	1.6986120
H	0.6640570	0.9032840	-1.8438620
H	-0.7841940	1.8280340	-1.3851650
H	0.8325920	2.3894250	-0.8688590
H	0.1167270	2.3743450	1.6037400
H	-1.5240560	1.9493000	1.0518790
H	-0.7229190	0.9536030	2.2876530
H	4.0291250	0.3783930	-0.8334750

Norpinic Acid – Gas Phase @ 298 K

C	-1.0626320	-0.2642760	-0.7805040
C	-0.0006910	-1.3859390	-0.6243580
C	0.8070230	-0.4983030	0.3443420
C	-0.0140150	0.7647740	-0.1605810
C	0.6885590	1.5299030	-1.2877040
C	-0.4975390	1.7210720	0.9283920
H	-1.3782680	-0.0085640	-1.8021980
H	0.5563530	-1.5637360	-1.5544830
H	-0.3633020	-2.3382150	-0.2159560
H	0.5356680	-0.7120990	1.3923990
H	-0.9941510	1.1896030	1.7548880
H	0.3539980	2.2855980	1.3452540
H	-1.2060440	2.4584270	0.5170810
H	-0.0114020	2.2470220	-1.7455760
H	1.5503300	2.0970640	-0.8995340
H	1.0601390	0.8587350	-2.0762390
C	2.3114360	-0.4531800	0.1782010
O	2.9211150	-0.8935550	-0.7787120
O	3.0004720	0.1903990	1.1796490
C	-2.2782530	-0.4619140	0.0854950
O	-3.3574120	0.2325550	-0.3862360
O	-2.3293390	-1.1235040	1.1159520
H	2.3794590	0.4544870	1.8866170
H	-4.0848020	0.0717050	0.2528280

Norpinic Acid – Gas Phase @ 373 K

C	-1.0626320	-0.2642760	-0.7805040
C	-0.0006910	-1.3859390	-0.6243580
C	0.8070230	-0.4983030	0.3443420
C	-0.0140150	0.7647740	-0.1605810

C	0.6885590	1.5299030	-1.2877040
C	-0.4975390	1.7210720	0.9283920
H	-1.3782680	-0.0085640	-1.8021980
H	0.5563530	-1.5637360	-1.5544830
H	-0.3633020	-2.3382150	-0.2159560
H	0.5356680	-0.7120990	1.3923990
H	-0.9941510	1.1896030	1.7548880
H	0.3539980	2.2855980	1.3452540
H	-1.2060440	2.4584270	0.5170810
H	-0.0114020	2.2470220	-1.7455760
H	1.5503300	2.0970640	-0.8995340
H	1.0601390	0.8587350	-2.0762390
C	2.3114360	-0.4531800	0.1782010
O	2.9211150	-0.8935550	-0.7787120
O	3.0004720	0.1903990	1.1796490
C	-2.2782530	-0.4619140	0.0854950
O	-3.3574120	0.2325550	-0.3862360
O	-2.3293390	-1.1235040	1.1159520
H	2.3794590	0.4544870	1.8866170
H	-4.0848020	0.0717050	0.2528280

Water – Gas Phase @ 298 K

O	0.0000000	0.0000000	0.1183600
H	0.0000000	0.7713820	-0.4734380
H	0.0000000	-0.7713820	-0.4734380

Water – Gas Phase @ 373 K

O	0.0000000	0.0000000	0.1183600
H	0.0000000	-0.7713820	-0.4734380
H	0.0000000	0.7713820	-0.4734380

cis-Pinic Acid – Gas Phase @ 298 K

C	-2.6419900	-0.4665740	-0.1083180
C	-1.2797990	-0.3022900	-0.7244650
C	-0.2542160	-1.3861450	-0.2923470
C	0.3131210	-0.4043200	0.7639820
C	-0.3783820	0.7918800	0.0135000
C	1.8036030	-0.3731210	1.1441260
C	2.8059670	-0.3711330	0.0095480
C	0.5070710	1.5002780	-1.0190210
C	-1.0767550	1.8179230	0.9072740
O	-2.9126580	-1.1043080	0.9027430
O	-3.5970960	0.2332040	-0.7974170
O	3.7605510	0.5965640	0.1732640

O	2.8289640	-1.1452540	-0.9386540
H	-1.3925600	-0.1213680	-1.8035320
H	0.4626780	-1.6062780	-1.0940860
H	-0.6801290	-2.3228460	0.0938230
H	-0.2399950	-0.5578510	1.7058570
H	2.0091020	0.4801190	1.8087070
H	2.0237100	-1.2873530	1.7247920
H	0.9962150	0.7934230	-1.7061990
H	-0.1020130	2.1903430	-1.6255280
H	1.2909950	2.0964110	-0.5233250
H	-0.3273030	2.4122980	1.4565670
H	-1.6857660	2.5185310	0.3127610
H	-1.7312000	1.3360840	1.6504290
H	-4.4357660	0.0972110	-0.3064540
H	4.3822190	0.4906420	-0.5789820

***cis*-Pinic Acid – Gas Phase @ 373 K**

C	-2.6419900	-0.4665740	-0.1083180
C	-1.2797990	-0.3022900	-0.7244650
C	-0.2542160	-1.3861450	-0.2923470
C	0.3131210	-0.4043200	0.7639820
C	-0.3783820	0.7918800	0.0135000
C	1.8036030	-0.3731210	1.1441260
C	2.8059670	-0.3711330	0.0095480
C	0.5070710	1.5002780	-1.0190210
C	-1.0767550	1.8179230	0.9072740
O	-2.9126580	-1.1043080	0.9027430
O	-3.5970960	0.2332040	-0.7974170
O	3.7605510	0.5965640	0.1732640
O	2.8289640	-1.1452540	-0.9386540
H	-1.3925600	-0.1213680	-1.8035320
H	0.4626780	-1.6062780	-1.0940860
H	-0.6801290	-2.3228460	0.0938230
H	-0.2399950	-0.5578510	1.7058570
H	2.0091020	0.4801190	1.8087070
H	2.0237100	-1.2873530	1.7247920
H	0.9962150	0.7934230	-1.7061990
H	-0.1020130	2.1903430	-1.6255280
H	1.2909950	2.0964110	-0.5233250
H	-0.3273030	2.4122980	1.4565670
H	-1.6857660	2.5185310	0.3127610
H	-1.7312000	1.3360840	1.6504290
H	-4.4357660	0.0972110	-0.3064540
H	4.3822190	0.4906420	-0.5789820

Pinonaldehyde – Gas Phase @ 298 K

C	-2.3756330	0.5604230	-0.5591350
C	-2.6156640	-0.9212570	-0.3757890
O	2.8843950	-0.2103820	-1.1378510
C	2.1461090	-0.6719690	-0.2680550
C	2.6969070	-1.4611470	0.9057280
C	0.6452040	-0.4542350	-0.3021050
C	0.0104180	0.1204780	-1.5862610
C	-0.9111890	1.0278770	-0.7183200
C	0.0631970	0.7966150	0.5019160
C	-0.5348400	0.5072960	1.8781560
C	1.0685760	1.9540890	0.5928020
O	-3.2663600	-1.4131830	0.5377810
H	-2.8789410	1.0976770	0.2602300
H	-2.8988610	0.8229190	-1.5007440
H	-2.1872020	-1.5852170	-1.1702530
H	3.7926660	-1.4050970	0.9215580
H	2.2827780	-1.0927640	1.8587800
H	2.3879870	-2.5168680	0.8178940
H	0.1349850	-1.3676430	0.0523310
H	-0.4671810	-0.5953550	-2.2720240
H	0.7543910	0.6967920	-2.1548780
H	-0.9447290	2.0837920	-1.0369510
H	-1.2589530	-0.3198340	1.8669400
H	0.2608620	0.2494700	2.5971050
H	-1.0494020	1.3994630	2.2733650
H	0.5524820	2.8677270	0.9311340
H	1.8700530	1.7350340	1.3174970
H	1.5462680	2.1693900	-0.3750450

Pinonaldehyde – Gas Phase @ 373 K

C	-2.3756330	0.5604230	-0.5591350
C	-2.6156640	-0.9212570	-0.3757890
O	2.8843950	-0.2103820	-1.1378510
C	2.1461090	-0.6719690	-0.2680550
C	2.6969070	-1.4611470	0.9057280
C	0.6452040	-0.4542350	-0.3021050
C	0.0104180	0.1204780	-1.5862610
C	-0.9111890	1.0278770	-0.7183200
C	0.0631970	0.7966150	0.5019160
C	-0.5348400	0.5072960	1.8781560
C	1.0685760	1.9540890	0.5928020
O	-3.2663600	-1.4131830	0.5377810
H	-2.8789410	1.0976770	0.2602300
H	-2.8988610	0.8229190	-1.5007440
H	-2.1872020	-1.5852170	-1.1702530
H	3.7926660	-1.4050970	0.9215580

H	2.2827780	-1.0927640	1.8587800
H	2.3879870	-2.5168680	0.8178940
H	0.1349850	-1.3676430	0.0523310
H	-0.4671810	-0.5953550	-2.2720240
H	0.7543910	0.6967920	-2.1548780
H	-0.9447290	2.0837920	-1.0369510
H	-1.2589530	-0.3198340	1.8669400
H	0.2608620	0.2494700	2.5971050
H	-1.0494020	1.3994630	2.2733650
H	0.5524820	2.8677270	0.9311340
H	1.8700530	1.7350340	1.3174970
H	1.5462680	2.1693900	-0.3750450

***cis*-Pinonic Acid – Gas Phase @ 298 K**

C	-2.8814240	-0.0568880	-0.3913670
C	-1.8816480	-0.9173280	0.3498780
C	-0.4247260	-0.7022310	-0.0459140
C	0.6324140	-1.5764030	0.6758990
C	1.5964000	-0.3654290	0.7388160
C	0.3585240	0.5925760	0.3924710
C	0.5476270	1.6518910	-0.6951250
C	-0.1746260	1.2364130	1.6778250
O	-2.6350560	0.7568240	-1.2702680
O	-4.1584180	-0.2959850	0.0400060
H	-4.7376810	0.2893490	-0.4929930
H	-2.0408900	-0.7614130	1.4313180
H	-2.1641870	-1.9710750	0.1705750
H	-0.3223300	-0.8191570	-1.1366130
H	1.0071440	-2.4451810	0.1161630
H	0.3086820	-1.8954070	1.6793520
H	2.0431970	-0.1420050	1.7226380
H	-0.3160400	0.5034130	2.4887410
H	0.5322100	2.0000690	2.0420780
H	-1.1396360	1.7385430	1.4965810
H	-0.4286640	2.0835740	-0.9632600
H	1.2041810	2.4701410	-0.3536290
H	0.9773440	1.2213910	-1.6128980
C	2.6892840	-0.3723630	-0.3147890
O	2.6442630	-1.1099530	-1.2997220
C	3.8468140	0.5866370	-0.0989200
H	4.4638160	0.6478630	-1.0043070
H	3.4862480	1.5880760	0.1857360
H	4.4684580	0.2234850	0.7377530

***cis*-Pinonic Acid – Gas Phase @ 373 K**

C	-2.8814240	-0.0568880	-0.3913670
C	-1.8816480	-0.9173280	0.3498780
C	-0.4247260	-0.7022310	-0.0459140
C	0.6324140	-1.5764030	0.6758990
C	1.5964000	-0.3654290	0.7388160
C	0.3585240	0.5925760	0.3924710
C	0.5476270	1.6518910	-0.6951250
C	-0.1746260	1.2364130	1.6778250
O	-2.6350560	0.7568250	-1.2702680
O	-4.1584180	-0.2959850	0.0400060
H	-4.7376810	0.2893490	-0.4929930
H	-2.0408900	-0.7614130	1.4313180
H	-2.1641870	-1.9710750	0.1705750
H	-0.3223300	-0.8191570	-1.1366130
H	1.0071440	-2.4451810	0.1161630
H	0.3086820	-1.8954070	1.6793520
H	2.0431970	-0.1420050	1.7226380
H	-0.3160400	0.5034130	2.4887410
H	0.5322100	2.0000690	2.0420780
H	-1.1396360	1.7385430	1.4965810
H	-0.4286640	2.0835740	-0.9632600
H	1.2041810	2.4701410	-0.3536290
H	0.9773440	1.2213910	-1.6128980
C	2.6892840	-0.3723630	-0.3147890
O	2.6442630	-1.1099530	-1.2997220
C	3.8468140	0.5866360	-0.0989200
H	4.4638160	0.6478630	-1.0043080
H	3.4862480	1.5880760	0.1857370
H	4.4684580	0.2234850	0.7377530

Hemi-acetal Monomer 1 – Gas Phase @ 298 K

O	-2.1698640	-1.6429390	0.2243940
C	-2.9252680	-0.7118040	0.0201360
C	-2.5394260	0.6905890	-0.4442290
C	-1.0630810	0.9952640	-0.7364140
C	-0.2326230	-0.0617770	-1.5226280
C	0.6195640	-0.3502590	-0.2645130
C	0.0019000	0.9531530	0.4286490
C	0.9212050	2.1793210	0.3446920
C	-0.4842210	0.7533240	1.8639490
C	2.1128500	-0.3964630	-0.4053350
O	2.7243830	0.0928580	-1.3620770
O	-4.2725340	-0.8987980	0.2085460
C	2.9229500	-1.0502140	0.7075890

O	4.3073290	-0.9111140	0.4942290
H	-2.9232110	1.4082200	0.3060310
H	-3.1191680	0.8892570	-1.3661510
H	-1.0629920	1.9851230	-1.2245910
H	0.3688630	0.3868580	-2.3261630
H	-0.7811260	-0.9280400	-1.9167200
H	0.2582100	-1.2395520	0.2742990
H	1.3214620	2.3270730	-0.6700360
H	0.3596030	3.0855720	0.6272220
H	1.7786630	2.0899860	1.0320020
H	0.3756850	0.6283210	2.5433110
H	-1.0446640	1.6364680	2.2163360
H	-1.1224980	-0.1351210	1.9692450
H	-4.7604050	-0.0757390	0.0094430
H	2.6269190	-0.6011730	1.6780650
H	2.6309420	-2.1203160	0.7577700
H	4.3761000	-0.4638050	-0.3821660

Hemi-acetal Monomer 1 – Gas Phase @ 373 K

Symbol	X	Y	Z
O	-2.1698640	-1.6429390	0.2243940
C	-2.9252680	-0.7118040	0.0201360
C	-2.5394260	0.6905890	-0.4442290
C	-1.0630810	0.9952640	-0.7364140
C	-0.2326230	-0.0617770	-1.5226280
C	0.6195640	-0.3502590	-0.2645130
C	0.0019000	0.9531530	0.4286490
C	0.9212050	2.1793210	0.3446920
C	-0.4842210	0.7533240	1.8639490
C	2.1128500	-0.3964630	-0.4053350
O	2.7243830	0.0928580	-1.3620770
O	-4.2725340	-0.8987980	0.2085460
C	2.9229500	-1.0502140	0.7075890
O	4.3073290	-0.9111140	0.4942290
H	-2.9232110	1.4082200	0.3060310
H	-3.1191680	0.8892570	-1.3661510
H	-1.0629920	1.9851230	-1.2245910
H	0.3688630	0.3868580	-2.3261630
H	-0.7811260	-0.9280400	-1.9167200
H	0.2582100	-1.2395520	0.2742990
H	1.3214620	2.3270730	-0.6700360
H	0.3596030	3.0855720	0.6272220
H	1.7786630	2.0899860	1.0320020
H	0.3756850	0.6283210	2.5433110
H	-1.0446640	1.6364680	2.2163360
H	-1.1224980	-0.1351210	1.9692450

H	-4.7604050	-0.0757390	0.0094430
H	2.6269190	-0.6011730	1.6780650
H	2.6309420	-2.1203160	0.7577700
H	4.3761000	-0.4638050	-0.3821660

Hydroperoxide Monomer – Gas Phase @ 298 K

C	-2.1937600	-1.1298020	-0.3286090
C	-0.8714540	-0.4059830	-0.1447410
C	-0.0492220	-0.5087130	1.1714190
C	0.3381250	0.9952200	1.0144800
C	-0.8305660	1.1625200	-0.0417580
C	-0.5600910	1.9315030	-1.3355530
C	-2.0775400	1.7383420	0.6488410
C	1.7813220	1.3167870	0.5862980
C	2.4902080	0.4113820	-0.4311800
O	2.9621550	-0.7386860	0.2892710
O	3.7752310	-1.5159490	-0.6699100
C	-2.3724500	-2.4541410	0.3926410
O	-3.0750240	-0.6685110	-1.0542680
H	-0.2458820	-0.7306410	-0.9989190
H	0.7798970	-1.2295600	1.1904970
H	-0.6855210	-0.6786710	2.0537250
H	0.1416040	1.5924980	1.9218130
H	0.3220870	1.5579070	-1.8779360
H	-1.4270570	1.8416160	-2.0090730
H	-0.4016140	3.0044820	-1.1329170
H	-1.9066240	2.7975880	0.9038730
H	-2.9593310	1.6728030	-0.0054150
H	-2.3114080	1.2059800	1.5859810
H	1.8062110	2.3418810	0.1764880
H	2.4215830	1.3412040	1.4857460
H	1.8348870	0.0883850	-1.2599000
H	3.3597850	0.9375830	-0.8629980
H	3.2851950	-2.3640560	-0.6523060
H	-3.2502010	-2.9810580	-0.0023690
H	-1.4716260	-3.0827240	0.3006910
H	-2.5183130	-2.2727480	1.4712540

Hydroperoxide Monomer – Gas Phase @ 373 K

C	-2.1937600	-1.1298020	-0.3286090
C	-0.8714540	-0.4059830	-0.1447410
C	-0.0492220	-0.5087130	1.1714190
C	0.3381250	0.9952200	1.0144800
C	-0.8305660	1.1625200	-0.0417580
C	-0.5600910	1.9315030	-1.3355530

C	-2.0775400	1.7383420	0.6488410
C	1.7813220	1.3167870	0.5862980
C	2.4902080	0.4113820	-0.4311800
O	2.9621550	-0.7386860	0.2892710
O	3.7752310	-1.5159490	-0.6699100
C	-2.3724500	-2.4541410	0.3926410
O	-3.0750240	-0.6685110	-1.0542680
H	-0.2458820	-0.7306410	-0.9989190
H	0.7798970	-1.2295600	1.1904970
H	-0.6855210	-0.6786710	2.0537250
H	0.1416040	1.5924980	1.9218130
H	0.3220870	1.5579070	-1.8779360
H	-1.4270570	1.8416160	-2.0090730
H	-0.4016140	3.0044820	-1.1329170
H	-1.9066240	2.7975880	0.9038730
H	-2.9593310	1.6728030	-0.0054150
H	-2.3114080	1.2059800	1.5859810
H	1.8062110	2.3418810	0.1764880
H	2.4215830	1.3412040	1.4857460
H	1.8348870	0.0883850	-1.2599000
H	3.3597850	0.9375830	-0.8629980
H	3.2851950	-2.3640560	-0.6523060
H	-3.2502010	-2.9810580	-0.0023690
H	-1.4716260	-3.0827240	0.3006910
H	-2.5183130	-2.2727480	1.4712540

2,2-dimethyl-3-formyl-cyclobutyl-methanoic acid - Gas Phase @ 298 K

C	2.3789130	0.0837110	-0.0418070
C	1.0692420	-0.0916760	0.7253960
C	0.2123660	-1.3238700	0.3010720
C	-0.7582830	-0.3793590	-0.4387440
C	-0.1403880	0.8514920	0.3543680
C	-0.9398370	1.2024420	1.6171180
C	0.1214580	2.1072840	-0.4765290
C	-2.2330420	-0.6278840	-0.2946360
O	-2.7638890	-1.4319250	0.4611950
O	-2.9673700	0.2001850	-1.1041540
H	1.3368530	-0.0508450	1.7938980
H	-0.2742110	-1.8187070	1.1530550
H	0.7017380	-2.0831200	-0.3268500
H	-0.5034400	-0.2793020	-1.5042610
H	-3.9079620	-0.0091470	-0.9192810
H	-1.1739870	0.3132470	2.2230020
H	-0.3604430	1.8985790	2.2455960
H	-1.8910010	1.6957210	1.3580780

H	-0.8359960	2.5528100	-0.7923870
H	0.6608680	2.8662250	0.1154480
H	0.7097170	1.8823220	-1.3776900
O	3.4003330	-0.7841410	0.4379690
O	2.1359230	-0.1401380	-1.4305240
H	3.0473300	-1.6950040	0.4036660
H	2.9937850	-0.0527040	-1.8859590
H	2.7942060	1.0952300	0.1203700

2,2-dimethyl-3-formyl-cyclobutyl-methanoic acid - Gas Phase @ 373 K

C	2.3789130	0.0837110	-0.0418070
C	1.0692420	-0.0916760	0.7253960
C	0.2123660	-1.3238700	0.3010720
C	-0.7582830	-0.3793590	-0.4387440
C	-0.1403880	0.8514920	0.3543680
C	-0.9398370	1.2024420	1.6171180
C	0.1214580	2.1072840	-0.4765290
C	-2.2330420	-0.6278840	-0.2946360
O	-2.7638890	-1.4319250	0.4611950
O	-2.9673700	0.2001850	-1.1041540
H	1.3368530	-0.0508450	1.7938980
H	-0.2742110	-1.8187070	1.1530550
H	0.7017380	-2.0831200	-0.3268500
H	-0.5034400	-0.2793020	-1.5042610
H	-3.9079620	-0.0091470	-0.9192810
H	-1.1739870	0.3132470	2.2230020
H	-0.3604430	1.8985790	2.2455960
H	-1.8910010	1.6957210	1.3580780
H	-0.8359960	2.5528100	-0.7923870
H	0.6608680	2.8662250	0.1154480
H	0.7097170	1.8823220	-1.3776900
O	3.4003330	-0.7841410	0.4379690
O	2.1359230	-0.1401380	-1.4305240
H	3.0473300	-1.6950040	0.4036660
H	2.9937850	-0.0527040	-1.8859590
H	2.7942060	1.0952300	0.1203700

Terpenylic Acid - Gas Phase @ 298 K

C	0.7171420	1.0133160	-0.0804370
C	-0.0124620	1.0985130	-1.4245980
C	0.9440600	2.3970700	0.5216160
O	2.0514830	0.4381630	-0.3472780
C	0.1096990	-0.0047540	0.9357470
C	0.7333840	-1.3350200	0.4963780

C	2.0758300	-0.9092790	-0.0829440
C	-1.4163440	0.0522760	1.1748120
C	-2.3626800	-0.3117450	0.0465790
O	-3.2180740	0.4244250	-0.4221200
O	-2.2057060	-1.6037650	-0.3776780
O	3.0566610	-1.5924480	-0.3014840
H	0.6084780	1.6636550	-2.1349530
H	-0.1920240	0.1018320	-1.8559160
H	-0.9781240	1.6151460	-1.3229540
H	-0.0188050	2.8621010	0.7850180
H	1.5644170	2.3308940	1.4278170
H	1.4526350	3.0541550	-0.1990640
H	0.5556220	0.2532890	1.9138270
H	0.1495480	-1.8400080	-0.2898810
H	0.8822800	-2.0597070	1.3085900
H	-1.6453040	-0.6340110	2.0087060
H	-1.7031550	1.0628010	1.4994620
H	-2.8822470	-1.7433900	-1.0750840

Terpenylic Acid - Gas Phase @ 373 K

C	0.7171420	1.0133160	-0.0804370
C	-0.0124620	1.0985130	-1.4245980
C	0.9440600	2.3970700	0.5216160
O	2.0514830	0.4381630	-0.3472780
C	0.1096990	-0.0047540	0.9357470
C	0.7333840	-1.3350200	0.4963780
C	2.0758300	-0.9092790	-0.0829440
C	-1.4163440	0.0522760	1.1748120
C	-2.3626800	-0.3117450	0.0465790
O	-3.2180740	0.4244250	-0.4221200
O	-2.2057060	-1.6037650	-0.3776780
O	3.0566610	-1.5924480	-0.3014840
H	0.6084780	1.6636550	-2.1349530
H	-0.1920240	0.1018320	-1.8559160
H	-0.9781240	1.6151460	-1.3229540
H	-0.0188050	2.8621010	0.7850180
H	1.5644170	2.3308940	1.4278170
H	1.4526350	3.0541550	-0.1990640
H	0.5556220	0.2532890	1.9138270
H	0.1495480	-1.8400080	-0.2898810
H	0.8822800	-2.0597070	1.3085900
H	-1.6453040	-0.6340110	2.0087060
H	-1.7031550	1.0628010	1.4994620
H	-2.8822470	-1.7433900	-1.0750840

Aldehyde Dimer – Gas Phase @ 298 K

C	-5.3339700	1.6083580	0.4465470
O	-4.8430120	2.8312700	-0.0702950
O	-4.9743690	0.4783180	-0.3346830
C	-3.5825320	0.1625870	-0.3149910
C	-3.1571510	-0.8135460	-1.4211280
C	-2.2585200	-1.5731620	-0.3991100
C	-3.0515630	-0.8369310	0.7800460
C	-0.7796470	-1.3050070	-0.4296230
O	0.0782080	-2.0830090	-0.0450720
O	-0.4963570	-0.0528730	-0.9647120
C	0.7849250	0.5614030	-0.9423040
O	1.0091060	1.3458280	-1.8400880
C	1.7041220	0.2621360	0.2054360
C	2.6336910	1.4634270	0.5584410
C	3.7976530	0.7973020	-0.2055510
C	3.0073480	-0.5751670	-0.2035480
C	-2.2294680	-0.2385920	1.9226090
C	-4.1436990	-1.7665080	1.3187030
C	3.3961060	-1.5021420	0.9529660
C	3.0140380	-1.3272680	-1.5314690
C	5.2002080	0.7676770	0.3383580
O	5.3238180	1.3727950	1.5599820
O	6.1509360	0.2368540	-0.2224330
H	-4.9206330	1.5459680	1.4679210
H	-6.4363010	1.5834620	0.4781820
H	-5.2483360	2.9685470	-0.9469890
H	-2.9856520	1.0899990	-0.3297390
H	-2.6669740	-0.3872240	-2.3059430
H	-4.0027030	-1.4428810	-1.7344490
H	-2.3688790	-2.6663500	-0.3728270
H	1.1542120	-0.1886550	1.0403390
H	2.8150210	1.5193540	1.6398840
H	2.3144120	2.4462950	0.1874740
H	3.8604570	1.1658740	-1.2411510
H	-1.4911490	0.4931620	1.5590150
H	-2.8882110	0.2847990	2.6348060
H	-1.6931130	-1.0231000	2.4817750
H	-3.6908320	-2.5848990	1.9013940
H	-4.8310000	-1.2157010	1.9803050
H	-4.7481520	-2.2073490	0.5120240
H	3.4300550	-0.9710520	1.9177900
H	2.6613490	-2.3173890	1.0344980
H	4.3888210	-1.9444520	0.7716160
H	4.0360200	-1.6810420	-1.7422730

H	2.3442550	-2.1998470	-1.4879990
H	2.7035840	-0.6844890	-2.3694220
H	6.2678560	1.2760870	1.8098910

Aldehyde Dimer – Gas Phase @ 373 K

C	-5.3339700	1.6083580	0.4465470
O	-4.8430120	2.8312700	-0.0702950
O	-4.9743690	0.4783180	-0.3346830
C	-3.5825320	0.1625870	-0.3149910
C	-3.1571510	-0.8135460	-1.4211280
C	-2.2585200	-1.5731620	-0.3991100
C	-3.0515630	-0.8369310	0.7800460
C	-0.7796470	-1.3050070	-0.4296230
O	0.0782080	-2.0830090	-0.0450720
O	-0.4963570	-0.0528730	-0.9647120
C	0.7849250	0.5614030	-0.9423040
O	1.0091060	1.3458280	-1.8400880
C	1.7041220	0.2621360	0.2054360
C	2.6336910	1.4634270	0.5584410
C	3.7976530	0.7973020	-0.2055510
C	3.0073480	-0.5751670	-0.2035480
C	-2.2294680	-0.2385920	1.9226090
C	-4.1436990	-1.7665080	1.3187030
C	3.3961060	-1.5021420	0.9529660
C	3.0140380	-1.3272680	-1.5314690
C	5.2002080	0.7676770	0.3383580
O	5.3238180	1.3727950	1.5599820
O	6.1509360	0.2368540	-0.2224330
H	-4.9206330	1.5459680	1.4679210
H	-6.4363010	1.5834620	0.4781820
H	-5.2483360	2.9685470	-0.9469890
H	-2.9856520	1.0899990	-0.3297390
H	-2.6669740	-0.3872240	-2.3059430
H	-4.0027030	-1.4428810	-1.7344490
H	-2.3688790	-2.6663500	-0.3728270
H	1.1542120	-0.1886550	1.0403390
H	2.8150210	1.5193540	1.6398840
H	2.3144120	2.4462950	0.1874740
H	3.8604570	1.1658740	-1.2411510
H	-1.4911490	0.4931620	1.5590150
H	-2.8882110	0.2847990	2.6348060
H	-1.6931130	-1.0231000	2.4817750
H	-3.6908320	-2.5848990	1.9013940
H	-4.8310000	-1.2157010	1.9803050
H	-4.7481520	-2.2073490	0.5120240
H	3.4300550	-0.9710520	1.9177900

H	2.6613490	-2.3173890	1.0344980
H	4.3888210	-1.9444520	0.7716160
H	4.0360200	-1.6810420	-1.7422730
H	2.3442550	-2.1998470	-1.4879990
H	2.7035840	-0.6844890	-2.3694220
H	6.2678560	1.2760870	1.8098910

***cis*-Pinic Acid Dimer – Gas Phase @ 298 K**

O	6.2006380	-1.6981730	-0.5031050
C	6.9472640	-0.8432060	-0.0676810
C	6.5466400	0.4166040	0.6962070
C	5.0569740	0.6908970	0.9461590
C	4.1473370	-0.4946770	1.3911060
C	3.4007140	-0.4342300	0.0414300
C	4.0882200	0.9647270	-0.2725260
C	3.1802340	2.1641440	0.0350000
C	4.6805520	1.0993240	-1.6749390
C	1.8994730	-0.4686890	0.0434790
O	8.3019800	-0.9928510	-0.2458730
O	1.2240700	-0.4446610	1.0953420
O	1.3652670	-0.4921310	-1.1715950
H	6.9973970	1.2834640	0.1761050
H	7.0565480	0.3621930	1.6775070
H	5.0337230	1.5342200	1.6578570
H	3.4948250	-0.2341630	2.2364390
H	4.6480990	-1.4490240	1.6024410
H	3.7745840	-1.1863250	-0.6681230
H	2.7169290	2.0860900	1.0315360
H	3.7669890	3.0976580	0.0071880
H	2.3724970	2.2518740	-0.7096610
H	3.8692740	1.1430980	-2.4195270
H	5.2662760	2.0301540	-1.7699230
H	5.3242330	0.2484210	-1.9392740
H	8.7796350	-0.2365610	0.1476590
H	0.3340850	-0.4777630	-1.1143880
O	-6.2006520	-1.6981620	0.5031010
C	-6.9472720	-0.8431950	0.0676690
C	-6.5466360	0.4166190	-0.6962090
C	-5.0569670	0.6909010	-0.9461550
C	-4.1473370	-0.4946790	-1.3911040
C	-3.4007140	-0.4342420	-0.0414280
C	-4.0882150	0.9647170	0.2725350
C	-3.1802220	2.1641330	-0.0349770
C	-4.6805480	1.0993050	1.6749490
C	-1.8994730	-0.4687020	-0.0434780
O	-8.3019910	-0.9928400	0.2458400

O	-1.2240710	-0.4446430	-1.0953410
O	-1.3652670	-0.4921780	1.1715940
H	-6.9973870	1.2834770	-0.1760970
H	-7.0565440	0.3622230	-1.6775090
H	-5.0337060	1.5342270	-1.6578480
H	-3.4948240	-0.2341670	-2.2364360
H	-4.6481070	-1.4490200	-1.6024410
H	-3.7745850	-1.1863380	0.6681230
H	-2.7169150	2.0860860	-1.0315120
H	-3.7669750	3.0976490	-0.0071600
H	-2.3724880	2.2518550	0.7096870
H	-3.8692710	1.1430720	2.4195380
H	-5.2662710	2.0301360	1.7699380
H	-5.3242320	0.2484010	1.9392750
H	-8.7796390	-0.2365500	-0.1476990
H	-0.3340850	-0.4778000	1.1143870

***cis*-Pinic Acid Dimer – Gas Phase @ 373 K**

O	6.2006450	-1.6981630	-0.5031220
C	6.9472710	-0.8432080	-0.0676760
C	6.5466420	0.4166020	0.6962100
C	5.0569740	0.6908900	0.9461590
C	4.1473380	-0.4946880	1.3910960
C	3.4007150	-0.4342330	0.0414210
C	4.0882230	0.9647250	-0.2725290
C	3.1802380	2.1641430	0.0349960
C	4.6805590	1.0993240	-1.6749400
C	1.8994730	-0.4686850	0.0434720
O	8.3019890	-0.9928650	-0.2458400
O	1.2240720	-0.4446470	1.0953350
O	1.3652660	-0.4921330	-1.1716010
H	6.9973970	1.2834620	0.1761060
H	7.0565490	0.3621960	1.6775110
H	5.0337180	1.5342090	1.6578610
H	3.4948270	-0.2341820	2.2364310
H	4.6481020	-1.4490350	1.6024230
H	3.7745800	-1.1863240	-0.6681370
H	2.7169310	2.0860880	1.0315310
H	3.7669960	3.0976560	0.0071880
H	2.3725040	2.2518770	-0.7096670
H	3.8692830	1.1431050	-2.4195300
H	5.2662890	2.0301510	-1.7699190
H	5.3242370	0.2484180	-1.9392760
H	8.7796430	-0.2365830	0.1477080
H	0.3340840	-0.4777540	-1.1143920
O	-6.2006450	-1.6981760	0.5030900

C	-6.9472700	-0.8432080	0.0676690
C	-6.5466420	0.4166080	-0.6962090
C	-5.0569740	0.6908990	-0.9461530
C	-4.1473360	-0.4946730	-1.3911050
C	-3.4007140	-0.4342350	-0.0414290
C	-4.0882250	0.9647180	0.2725390
C	-3.1802410	2.1641420	-0.0349690
C	-4.6805610	1.0992970	1.6749520
C	-1.8994730	-0.4686840	-0.0434790
O	-8.3019860	-0.9928550	0.2458510
O	-1.2240700	-0.4446180	-1.0953420
O	-1.3652660	-0.4921610	1.1715940
H	-6.9973990	1.2834640	-0.1761010
H	-7.0565470	0.3622060	-1.6775100
H	-5.0337170	1.5342270	-1.6578440
H	-3.4948250	-0.2341540	-2.2364360
H	-4.6481000	-1.4490170	-1.6024450
H	-3.7745790	-1.1863360	0.6681190
H	-2.7169320	2.0861020	-1.0315040
H	-3.7670000	3.0976540	-0.0071470
H	-2.3725070	2.2518660	0.7096960
H	-3.8692860	1.1430700	2.4195430
H	-5.2662930	2.0301220	1.7699430
H	-5.3242370	0.2483860	1.9392760
H	-8.7796400	-0.2365620	-0.1476760
H	-0.3340850	-0.4777810	1.1143850

Ester Dimer – Gas Phase @ 298 K

O	4.0119160	1.2547320	-1.9899870
C	4.6714500	1.1059260	-0.9684760
C	4.5102840	0.0011170	0.0397380
C	3.8592280	-1.2880410	-0.5393860
C	2.5060140	-0.8447240	0.0310090
C	3.2298580	0.1782360	0.9799050
C	3.5241750	-0.4032660	2.3665180
C	2.6117620	1.5727350	1.0879610
O	5.6454120	1.9930940	-0.5972550
O	1.7524010	-1.9063210	0.6355970
C	0.3840280	-1.6928910	0.7094800
O	-0.1725560	-1.8739460	-0.6259950
C	-1.4959100	-1.6423030	-0.9005570
O	-1.8837280	-1.8182210	-2.0456170
C	-2.3905030	-1.1372990	0.2148470
C	-3.9038070	-1.3056410	-0.0899220
C	-3.9940110	0.1748800	-0.5077080
C	-2.5958730	0.4485690	0.1906060

C	-5.1698150	0.9765100	-0.0200180
O	-5.9955650	0.6172120	0.8088610
O	-5.2046600	2.2205710	-0.5920660
C	-2.7269800	0.9850540	1.6204230
C	-1.6265670	1.2988780	-0.6286490
H	5.4486920	-0.1248050	0.5980910
H	4.2308340	-2.1864310	-0.0264590
H	3.9140130	-1.4280430	-1.6268280
H	1.8945800	-0.3320780	-0.7291710
H	3.9657650	-1.4094270	2.3108640
H	4.2235250	0.2529200	2.9092050
H	2.5995730	-0.4823100	2.9602040
H	1.6846780	1.5343780	1.6844340
H	3.2976710	2.2738650	1.5913010
H	2.3610860	1.9873690	0.0991540
H	5.6561380	2.6873740	-1.2908350
H	-0.0207640	-2.4620860	1.3855450
H	0.1342800	-0.6767480	1.0683580
H	-2.0655420	-1.5176860	1.1952210
H	-4.4906520	-1.5061400	0.8172900
H	-4.1494590	-2.0385310	-0.8688460
H	-3.8858290	0.3067040	-1.5948590
H	-5.9795400	2.6776860	-0.2001900
H	-3.4490630	0.4073800	2.2176430
H	-1.7508450	0.9467790	2.1318650
H	-3.0580300	2.0363760	1.6127660
H	-2.0273920	2.3203900	-0.7302770
H	-0.6422530	1.3764820	-0.1367940
H	-1.4772280	0.8931650	-1.6406130

Ester Dimer – Gas Phase @ 373 K

O	4.0119160	1.2547320	-1.9899870
C	4.6714500	1.1059260	-0.9684760
C	4.5102840	0.0011170	0.0397380
C	3.8592280	-1.2880410	-0.5393860
C	2.5060140	-0.8447240	0.0310090
C	3.2298580	0.1782360	0.9799050
C	3.5241750	-0.4032660	2.3665180
C	2.6117620	1.5727350	1.0879610
O	5.6454120	1.9930940	-0.5972550
O	1.7524010	-1.9063210	0.6355970
C	0.3840280	-1.6928910	0.7094800
O	-0.1725560	-1.8739460	-0.6259950
C	-1.4959100	-1.6423030	-0.9005570
O	-1.8837280	-1.8182210	-2.0456170
C	-2.3905030	-1.1372990	0.2148470

C	-3.9038070	-1.3056410	-0.0899220
C	-3.9940110	0.1748800	-0.5077080
C	-2.5958730	0.4485690	0.1906060
C	-5.1698150	0.9765100	-0.0200180
O	-5.9955650	0.6172120	0.8088610
O	-5.2046600	2.2205710	-0.5920660
C	-2.7269800	0.9850540	1.6204230
C	-1.6265670	1.2988780	-0.6286490
H	5.4486920	-0.1248050	0.5980910
H	4.2308340	-2.1864310	-0.0264590
H	3.9140130	-1.4280430	-1.6268280
H	1.8945800	-0.3320780	-0.7291710
H	3.9657650	-1.4094270	2.3108640
H	4.2235250	0.2529200	2.9092050
H	2.5995730	-0.4823100	2.9602040
H	1.6846780	1.5343780	1.6844340
H	3.2976710	2.2738650	1.5913010
H	2.3610860	1.9873690	0.0991540
H	5.6561380	2.6873740	-1.2908350
H	-0.0207640	-2.4620860	1.3855450
H	0.1342800	-0.6767480	1.0683580
H	-2.0655420	-1.5176860	1.1952210
H	-4.4906520	-1.5061400	0.8172900
H	-4.1494590	-2.0385310	-0.8688460
H	-3.8858290	0.3067040	-1.5948590
H	-5.9795400	2.6776860	-0.2001900
H	-3.4490630	0.4073800	2.2176430
H	-1.7508450	0.9467790	2.1318650
H	-3.0580300	2.0363760	1.6127660
H	-2.0273920	2.3203900	-0.7302770
H	-0.6422530	1.3764820	-0.1367940
H	-1.4772280	0.8931650	-1.6406130

Aldol Addition Dimer – Gas Phase @ 298 K

C	-5.0690920	1.5983090	0.1174410
C	-4.8200910	2.4778850	-1.0974770
O	-6.1707270	1.5922790	0.6687670
C	-3.9563760	0.7164140	0.6573250
C	-2.4933880	0.9595790	0.1870890
C	-2.5985310	-0.2698960	-0.7536050
C	-3.8951300	-0.7429440	0.0019850
C	-3.6205750	-1.7851930	1.0938540
C	-5.0675460	-1.1830080	-0.8746460
C	-1.4418440	-1.2327180	-0.9561550
O	-1.6521970	-2.4216830	-1.2014140
C	-0.0168330	-0.6751990	-0.9272740

C	0.8275860	-1.1224940	0.2970990
O	0.0635050	-0.7021890	1.4612480
C	2.2201030	-0.4545520	0.2423240
C	3.1847620	-0.6173120	1.4475710
C	3.7302300	0.8183330	1.1858110
C	2.4874370	1.1036590	0.2477030
C	2.7665890	1.7321990	-1.1222480
C	1.4687360	1.9664710	1.0094910
C	5.1539680	0.9704690	0.6299250
C	5.5854870	0.1081540	-0.5393330
O	6.5864740	0.7167230	-1.2476640
O	5.1753500	-1.0061460	-0.8357550
H	-4.1981880	3.3413260	-0.8046520
H	-4.2724370	1.9471890	-1.8925660
H	-5.7786260	2.8487220	-1.4816840
H	-4.1026500	0.6702150	1.7473910
H	-1.7749340	0.7904940	1.0011270
H	-2.2729380	1.9300630	-0.2829190
H	-2.8769870	0.0548030	-1.7759210
H	-2.7603640	-1.5004670	1.7203300
H	-4.5058570	-1.8812430	1.7430070
H	-3.4024890	-2.7660830	0.6458360
H	-4.8349610	-2.1532210	-1.3414850
H	-5.9857510	-1.2957430	-0.2763520
H	-5.2807980	-0.4639570	-1.6820410
H	0.4943980	-1.0331000	-1.8354240
H	-0.0423370	0.4246260	-0.9569910
H	0.4254070	-1.1743170	2.2330840
H	2.7293200	-0.8669820	-0.6448110
H	3.9039740	-1.4453280	1.3838260
H	2.6630980	-0.6682340	2.4181420
H	3.7034410	1.4571450	2.0854020
H	3.4753100	1.1401480	-1.7215410
H	1.8359350	1.8129240	-1.7082760
H	3.1735640	2.7525180	-1.0177210
H	1.8821950	2.9807720	1.1473940
H	0.5177860	2.0652580	0.4633960
H	1.2307620	1.5508140	1.9987550
H	5.3546980	2.0215890	0.3681490
H	5.8699040	0.7291650	1.4390220
H	6.8522780	0.0763970	-1.9422550
C	1.0131830	-2.6481120	0.3430420
H	0.0436800	-3.1622210	0.3801920
H	1.5568230	-3.0092580	-0.5430790
H	1.6054480	-2.9261590	1.2316670

Aldol Addition Dimer – Gas Phase @ 373 K

C	-5.0690920	1.5983090	0.1174410
C	-4.8200910	2.4778850	-1.0974770
O	-6.1707270	1.5922790	0.6687670
C	-3.9563760	0.7164140	0.6573250
C	-2.4933880	0.9595790	0.1870890
C	-2.5985310	-0.2698960	-0.7536050
C	-3.8951300	-0.7429440	0.0019850
C	-3.6205750	-1.7851930	1.0938540
C	-5.0675460	-1.1830080	-0.8746460
C	-1.4418440	-1.2327180	-0.9561550
O	-1.6521970	-2.4216830	-1.2014140
C	-0.0168330	-0.6751990	-0.9272740
C	0.8275860	-1.1224940	0.2970990
O	0.0635050	-0.7021890	1.4612480
C	2.2201030	-0.4545520	0.2423240
C	3.1847620	-0.6173120	1.4475710
C	3.7302300	0.8183330	1.1858110
C	2.4874370	1.1036590	0.2477030
C	2.7665890	1.7321990	-1.1222480
C	1.4687360	1.9664710	1.0094910
C	5.1539680	0.9704690	0.6299250
C	5.5854870	0.1081540	-0.5393330
O	6.5864740	0.7167230	-1.2476640
O	5.1753500	-1.0061460	-0.8357550
H	-4.1981880	3.3413260	-0.8046520
H	-4.2724370	1.9471890	-1.8925660
H	-5.7786260	2.8487220	-1.4816840
H	-4.1026500	0.6702150	1.7473910
H	-1.7749340	0.7904940	1.0011270
H	-2.2729380	1.9300630	-0.2829190
H	-2.8769870	0.0548030	-1.7759210
H	-2.7603640	-1.5004670	1.7203300
H	-4.5058570	-1.8812430	1.7430070
H	-3.4024890	-2.7660830	0.6458360
H	-4.8349610	-2.1532210	-1.3414850
H	-5.9857510	-1.2957430	-0.2763520
H	-5.2807980	-0.4639570	-1.6820410
H	0.4943980	-1.0331000	-1.8354240
H	-0.0423370	0.4246260	-0.9569910
H	0.4254070	-1.1743170	2.2330840
H	2.7293200	-0.8669820	-0.6448110
H	3.9039740	-1.4453280	1.3838260
H	2.6630980	-0.6682340	2.4181420
H	3.7034410	1.4571450	2.0854020
H	3.4753100	1.1401480	-1.7215410

H	1.8359350	1.8129240	-1.7082760
H	3.1735640	2.7525180	-1.0177210
H	1.8821950	2.9807720	1.1473940
H	0.5177860	2.0652580	0.4633960
H	1.2307620	1.5508140	1.9987550
H	5.3546980	2.0215890	0.3681490
H	5.8699040	0.7291650	1.4390220
H	6.8522780	0.0763970	-1.9422550
C	1.0131830	-2.6481120	0.3430420
H	0.0436800	-3.1622210	0.3801920
H	1.5568230	-3.0092580	-0.5430790
H	1.6054480	-2.9261590	1.2316670

Hemi-acetal Dimer – Gas Phase @ 298 K

O	-7.2528280	1.5059950	-0.3497440
C	-6.4273960	0.4125430	-0.2754120
O	-6.6796210	-0.4635530	0.5312550
C	-5.2770500	0.3612670	-1.2783330
C	-3.8945600	-0.0593770	-0.7466930
C	-3.7091490	-1.2786050	0.1925940
C	-2.5834370	-0.5165960	0.9529650
C	-3.0861690	0.8391960	0.2609680
C	-2.0307190	1.7499370	-0.3698830
C	-3.9475450	1.6320990	1.2508900
C	-1.1345030	-0.8439740	0.6812990
C	-0.7691020	-1.7416630	-0.5100640
O	-0.2526360	-0.3765690	1.4088400
O	0.5489970	-1.5342160	-0.9800160
C	1.5496590	-2.4154330	-0.4485840
O	1.5466500	-2.4182240	0.9649930
C	2.8789360	-1.9922190	-1.0801470
C	3.3677400	-0.5706220	-0.7880210
C	4.5371410	-0.0494180	-1.6630060
C	5.1373270	0.6855220	-0.4399870
C	4.2022680	-0.2118650	0.5041880
C	3.4479400	0.4999710	1.6290310
C	5.0077140	-1.3869230	1.0689490
C	4.8332340	2.1701770	-0.3828230
O	3.9400750	2.6859890	-1.0566780
C	5.6881930	3.0033440	0.5575710
H	-6.9275390	2.1262670	-1.0300250
H	-5.1725160	1.3219170	-1.8139920
H	-5.5920120	-0.3775580	-2.0377860
H	-3.2638380	-0.1914040	-1.6440660
H	-3.4536050	-2.2370470	-0.2841960
H	-4.5822530	-1.4395630	0.8378920

H	-2.6908410	-0.4836350	2.0479360
H	-1.3970150	1.2193210	-1.0981090
H	-2.5192860	2.5855640	-0.8991080
H	-1.3665560	2.1805940	0.3958070
H	-3.3074940	2.0706110	2.0330090
H	-4.4654310	2.4657730	0.7466820
H	-4.7052700	1.0076080	1.7469300
H	-0.9420030	-2.7943040	-0.2019670
H	-1.4503680	-1.5352760	-1.3530350
H	1.3110850	-3.4577330	-0.7487180
H	1.2373650	-1.5212730	1.2450140
H	3.6348770	-2.7358020	-0.7766000
H	2.7618020	-2.0962010	-2.1744880
H	2.5220780	0.1314010	-0.8664220
H	4.2596250	0.5923870	-2.5117670
H	5.1952520	-0.8607390	-2.0131840
H	6.2119120	0.5280850	-0.2446160
H	2.8359510	1.3337750	1.2520750
H	2.7747160	-0.2039290	2.1423980
H	4.1424900	0.8935090	2.3908890
H	5.7148070	-1.0314610	1.8371650
H	4.3342200	-2.1231960	1.5368510
H	5.5939980	-1.9034750	0.2915650
H	5.2524930	4.0027370	0.6834310
H	5.8032470	2.5102750	1.5360490
H	6.7018950	3.1032280	0.1321770

Hemi-acetal Dimer – Gas Phase @ 373 K

O	-7.2528330	1.5059840	-0.3497160
C	-6.4274030	0.4125300	-0.2753850
O	-6.6796180	-0.4635570	0.5312940
C	-5.2770710	0.3612410	-1.2783220
C	-3.8945720	-0.0593890	-0.7466960
C	-3.7091430	-1.2786000	0.1926100
C	-2.5834270	-0.5165720	0.9529570
C	-3.0861700	0.8392050	0.2609390
C	-2.0307280	1.7499350	-0.3699440
C	-3.9475350	1.6321280	1.2508540
C	-1.1344940	-0.8439510	0.6812880
C	-0.7691010	-1.7416640	-0.5100600
O	-0.2526230	-0.3765270	1.4088110
O	0.5489940	-1.5342300	-0.9800240
C	1.5496570	-2.4154390	-0.4485770
O	1.5466350	-2.4182180	0.9649990
C	2.8789360	-1.9922250	-1.0801360
C	3.3677400	-0.5706270	-0.7880130

C	4.5371410	-0.0494270	-1.6629990
C	5.1373300	0.6855150	-0.4399810
C	4.2022670	-0.2118680	0.5041960
C	3.4479410	0.4999750	1.6290360
C	5.0077100	-1.3869270	1.0689600
C	4.8332400	2.1701710	-0.3828220
O	3.9400790	2.6859820	-1.0566750
C	5.6882070	3.0033400	0.5575640
H	-6.9275550	2.1262450	-1.0300110
H	-5.1725500	1.3218810	-1.8140010
H	-5.5920420	-0.3775990	-2.0377570
H	-3.2638630	-0.1914270	-1.6440770
H	-3.4535960	-2.2370470	-0.2841690
H	-4.5822380	-1.4395550	0.8379190
H	-2.6908250	-0.4835910	2.0479280
H	-1.3970330	1.2193030	-1.0981670
H	-2.5193020	2.5855500	-0.8991800
H	-1.3665560	2.1806080	0.3957290
H	-3.3074760	2.0706550	2.0329580
H	-4.4654260	2.4657930	0.7466350
H	-4.7052540	1.0076470	1.7469150
H	-0.9420070	-2.7942980	-0.2019440
H	-1.4503720	-1.5352870	-1.3530320
H	1.3110900	-3.4577420	-0.7487010
H	1.2373790	-1.5212550	1.2450090
H	3.6348770	-2.7358060	-0.7765870
H	2.7618040	-2.0962080	-2.1744780
H	2.5220790	0.1313970	-0.8664150
H	4.2596260	0.5923770	-2.5117610
H	5.1952510	-0.8607500	-2.0131740
H	6.2119140	0.5280750	-0.2446100
H	2.8359520	1.3337770	1.2520760
H	2.7747170	-0.2039220	2.1424090
H	4.1424920	0.8935160	2.3908920
H	5.7148050	-1.0314630	1.8371750
H	4.3342160	-2.1231960	1.5368650
H	5.5939930	-1.9034820	0.2915780
H	5.2525160	4.0027380	0.6834140
H	5.8032540	2.5102790	1.5360470
H	6.7019100	3.1032090	0.1321710

Peroxyhemiacetal Dimer – Gas Phase @ 298 K

C	-3.0189670	2.7067080	1.1475730
C	-3.8320570	1.4264930	1.1303260
O	-4.9440330	1.3598200	1.6567950
C	-3.2118250	0.2107020	0.4633190

C	-2.2236920	0.3363480	-0.7304810
C	-2.8725690	-0.9321560	-1.3685210
C	-4.1020590	-0.7719270	-0.3820560
C	-4.6412650	-2.0071040	0.3406040
C	-5.2542170	-0.0505910	-1.0999810
C	-2.0602830	-2.2402540	-1.3405990
C	-1.1902610	-2.5628980	-0.1167610
O	0.0224600	-1.8136840	-0.2566850
O	0.7975910	-2.1136310	0.9870300
C	2.2231340	-1.9938900	0.6567610
O	2.8117020	-2.1818780	1.9300580
C	2.6382130	-3.1667070	-0.2182600
C	2.4970270	-0.5746390	0.1190130
C	2.4226340	-0.2166510	-1.3873780
C	3.5212330	0.8639120	-1.1552280
C	3.9203460	0.1063890	0.1756550
C	4.2412270	0.9289120	1.4272770
C	5.1002350	-0.8374650	-0.1109110
C	3.0449980	2.3295610	-1.0871550
C	1.7314360	2.6109800	-0.3500960
O	1.4229900	3.9787910	-0.6487540
O	0.1260080	4.2575360	0.0096130
H	-1.9665840	2.5127130	1.4105100
H	-2.9992330	3.1528560	0.1385710
H	-3.4668270	3.4239390	1.8472730
H	-2.7270430	-0.3502710	1.2857450
H	-1.1532450	0.2696350	-0.4933320
H	-2.3997160	1.2398090	-1.3343910
H	-3.1845690	-0.7811350	-2.4167950
H	-3.8573270	-2.5627780	0.8779220
H	-5.3988280	-1.7027470	1.0800700
H	-5.1230540	-2.7028130	-0.3676850
H	-5.7049940	-0.7214560	-1.8505270
H	-6.0350270	0.2552770	-0.3881020
H	-4.9065360	0.8526630	-1.6287350
H	-2.7545740	-3.0887250	-1.4738670
H	-1.3947180	-2.2633890	-2.2221110
H	-1.6782260	-2.2934100	0.8364550
H	-0.9511300	-3.6419820	-0.0867800
H	2.5239700	-1.4403690	2.4981200
H	3.7062560	-3.1255980	-0.4676580
H	2.4352070	-4.0979810	0.3284230
H	2.0514870	-3.1590190	-1.1468330
H	1.7989590	0.0782140	0.6744180
H	1.4474620	0.1039740	-1.7805220
H	2.7922920	-1.0345500	-2.0238470

H	4.3379690	0.8425920	-1.8974920
H	3.4090330	1.5814220	1.7321940
H	4.4766300	0.2637620	2.2748900
H	5.1256340	1.5673630	1.2623670
H	6.0264420	-0.2464160	-0.2085330
H	5.2416430	-1.5619450	0.7061730
H	4.9720470	-1.3958630	-1.0511910
H	3.8431740	2.9536220	-0.6493650
H	2.9085180	2.6824800	-2.1245850
H	0.9129570	1.9675500	-0.7179830
H	1.8173640	2.4857450	0.7435900
H	0.3811260	5.0468850	0.5305680

Peroxyhemiacetal Dimer – Gas Phase @ 373 K

C	-3.0189670	2.7067080	1.1475730
C	-3.8320570	1.4264930	1.1303260
O	-4.9440330	1.3598200	1.6567950
C	-3.2118250	0.2107020	0.4633190
C	-2.2236920	0.3363480	-0.7304810
C	-2.8725690	-0.9321560	-1.3685210
C	-4.1020590	-0.7719270	-0.3820560
C	-4.6412650	-2.0071040	0.3406040
C	-5.2542170	-0.0505910	-1.0999810
C	-2.0602830	-2.2402540	-1.3405990
C	-1.1902610	-2.5628980	-0.1167610
O	0.0224600	-1.8136840	-0.2566850
O	0.7975910	-2.1136310	0.9870300
C	2.2231340	-1.9938900	0.6567610
O	2.8117020	-2.1818780	1.9300580
C	2.6382130	-3.1667070	-0.2182600
C	2.4970270	-0.5746390	0.1190130
C	2.4226340	-0.2166510	-1.3873780
C	3.5212330	0.8639120	-1.1552280
C	3.9203460	0.1063890	0.1756550
C	4.2412270	0.9289120	1.4272770
C	5.1002350	-0.8374650	-0.1109110
C	3.0449980	2.3295610	-1.0871550
C	1.7314360	2.6109800	-0.3500960
O	1.4229900	3.9787910	-0.6487540
O	0.1260080	4.2575360	0.0096130
H	-1.9665840	2.5127130	1.4105100
H	-2.9992330	3.1528560	0.1385710
H	-3.4668270	3.4239390	1.8472730
H	-2.7270430	-0.3502710	1.2857450
H	-1.1532450	0.2696350	-0.4933320
H	-2.3997160	1.2398090	-1.3343910

H	-3.1845690	-0.7811350	-2.4167950
H	-3.8573270	-2.5627780	0.8779220
H	-5.3988280	-1.7027470	1.0800700
H	-5.1230540	-2.7028130	-0.3676850
H	-5.7049940	-0.7214560	-1.8505270
H	-6.0350270	0.2552770	-0.3881020
H	-4.9065360	0.8526630	-1.6287350
H	-2.7545740	-3.0887250	-1.4738670
H	-1.3947180	-2.2633890	-2.2221110
H	-1.6782260	-2.2934100	0.8364550
H	-0.9511300	-3.6419820	-0.0867800
H	2.5239700	-1.4403690	2.4981200
H	3.7062560	-3.1255980	-0.4676580
H	2.4352070	-4.0979810	0.3284230
H	2.0514870	-3.1590190	-1.1468330
H	1.7989590	0.0782140	0.6744180
H	1.4474620	0.1039740	-1.7805220
H	2.7922920	-1.0345500	-2.0238470
H	4.3379690	0.8425920	-1.8974920
H	3.4090330	1.5814220	1.7321940
H	4.4766300	0.2637620	2.2748900
H	5.1256340	1.5673630	1.2623670
H	6.0264420	-0.2464160	-0.2085330
H	5.2416430	-1.5619450	0.7061730
H	4.9720470	-1.3958630	-1.0511910
H	3.8431740	2.9536220	-0.6493650
H	2.9085180	2.6824800	-2.1245850
H	0.9129570	1.9675500	-0.7179830
H	1.8173640	2.4857450	0.7435900
H	0.3811260	5.0468850	0.5305680

Di(α -hydroxy) Ether Dimer – Gas Phase @ 298 K

C	-4.6941290	1.4496740	0.9948710
C	-3.4673130	0.7846820	0.4352560
C	-2.5047790	1.4988830	-0.5414360
C	-2.3948300	0.1810920	-1.3656760
C	-3.6996260	-0.3509020	-0.6437610
C	-3.7651760	-1.7762660	-0.0890590
C	-4.9264810	-0.0743000	-1.5261160
C	-1.0714500	-0.5625100	-1.1827190
O	-1.0574090	-1.8296280	-1.8699100
H	-1.8534570	-2.3187180	-1.5834080
H	-1.5709390	1.8796870	-0.1047310
H	-2.9939930	2.3066730	-1.1020200
H	-0.2741800	0.0139240	-1.6845330
H	-2.5240980	0.2998960	-2.4542330

H	-4.9297380	-0.7552400	-2.3930100
H	-5.8592960	-0.2374600	-0.9626690
H	-4.9362600	0.9577660	-1.9115100
H	-2.8753190	-2.0294340	0.5050630
H	-4.6483120	-1.8730520	0.5634940
H	-3.8896160	-2.5199940	-0.8981870
O	-4.8450180	2.7491860	0.5921760
O	-5.5118110	0.8981310	1.7228200
H	-2.9155890	0.3472530	1.2812870
O	-0.8014120	-0.7010370	0.2015310
C	0.4656390	-1.3220380	0.6204690
C	0.4196670	-1.1738720	2.1379940
O	0.4389430	-2.7158080	0.3413370
C	1.6411150	-0.6520090	-0.1188980
C	3.1506160	-0.9693380	0.2581560
C	3.1900110	0.4271190	0.9791960
C	1.9060850	0.8475130	0.2170760
C	3.9732900	-1.0113480	-1.0421010
C	3.5241120	-2.1869320	1.1085260
C	4.4572890	1.3024690	1.0002580
C	4.9185330	1.8836890	-0.3193520
O	4.2326210	2.5187730	-1.1102760
O	6.2526190	1.6663320	-0.5356510
H	6.4628230	2.1113790	-1.3849190
H	4.2573580	2.1770060	1.6458020
H	5.2902380	0.7505940	1.4623600
H	2.9326600	0.2531780	2.0386560
H	2.1243380	1.4493120	-0.6758160
H	1.1312710	1.3647140	0.8037200
H	1.4801280	-0.8488380	-1.1923370
H	-0.5433290	-1.5673210	2.4916820
H	1.2215040	-1.7513790	2.6115820
H	0.4993740	-0.1199780	2.4371750
H	3.7343520	-0.1763070	-1.7189060
H	5.0552220	-0.9849100	-0.8323280
H	3.7628470	-1.9486040	-1.5834310
H	3.2052740	-3.1226440	0.6246140
H	4.6190890	-2.2263180	1.2398310
H	3.0754480	-2.1625950	2.1112580
H	0.2352310	-2.7908520	-0.6162420
H	-5.6767330	3.0610410	1.0094360

Terpenylic Acid Dimer – Gas Phase @ 298 K

C	-4.6941290	1.4496740	0.9948710
C	-3.4673130	0.7846820	0.4352560

C	-2.5047790	1.4988830	-0.5414360
C	-2.3948300	0.1810920	-1.3656760
C	-3.6996260	-0.3509020	-0.6437610
C	-3.7651760	-1.7762660	-0.0890590
C	-4.9264810	-0.0743000	-1.5261160
C	-1.0714500	-0.5625100	-1.1827190
O	-1.0574090	-1.8296280	-1.8699100
H	-1.8534570	-2.3187180	-1.5834080
H	-1.5709390	1.8796870	-0.1047310
H	-2.9939930	2.3066730	-1.1020200
H	-0.2741800	0.0139240	-1.6845330
H	-2.5240980	0.2998960	-2.4542330
H	-4.9297380	-0.7552400	-2.3930100
H	-5.8592960	-0.2374600	-0.9626690
H	-4.9362600	0.9577660	-1.9115100
H	-2.8753190	-2.0294340	0.5050630
H	-4.6483120	-1.8730520	0.5634940
H	-3.8896160	-2.5199940	-0.8981870
O	-4.8450180	2.7491860	0.5921760
O	-5.5118110	0.8981310	1.7228200
H	-2.9155890	0.3472530	1.2812870
O	-0.8014120	-0.7010370	0.2015310
C	0.4656390	-1.3220380	0.6204690
C	0.4196670	-1.1738720	2.1379940
O	0.4389430	-2.7158080	0.3413370
C	1.6411150	-0.6520090	-0.1188980
C	3.1506160	-0.9693380	0.2581560
C	3.1900110	0.4271190	0.9791960
C	1.9060850	0.8475130	0.2170760
C	3.9732900	-1.0113480	-1.0421010
C	3.5241120	-2.1869320	1.1085260
C	4.4572890	1.3024690	1.0002580
C	4.9185330	1.8836890	-0.3193520
O	4.2326210	2.5187730	-1.1102760
O	6.2526190	1.6663320	-0.5356510
H	6.4628230	2.1113790	-1.3849190
H	4.2573580	2.1770060	1.6458020
H	5.2902380	0.7505940	1.4623600
H	2.9326600	0.2531780	2.0386560
H	2.1243380	1.4493120	-0.6758160
H	1.1312710	1.3647140	0.8037200
H	1.4801280	-0.8488380	-1.1923370
H	-0.5433290	-1.5673210	2.4916820
H	1.2215040	-1.7513790	2.6115820
H	0.4993740	-0.1199780	2.4371750
H	3.7343520	-0.1763070	-1.7189060

H	5.0552220	-0.9849100	-0.8323280
H	3.7628470	-1.9486040	-1.5834310
H	3.2052740	-3.1226440	0.6246140
H	4.6190890	-2.2263180	1.2398310
H	3.0754480	-2.1625950	2.1112580
H	0.2352310	-2.7908520	-0.6162420
H	-5.6767330	3.0610410	1.0094360

Terpenylic Acid Dimer – Gas Phase @ 373 K

C	-4.0552550	0.9164280	-0.8444120
C	-4.2408920	-0.5799570	-0.4359930
O	-4.8266480	1.6322420	0.1889770
C	-4.9724580	0.8694500	1.3234320
C	-4.3616510	-0.5047280	1.0913530
C	-4.6962740	1.2522630	-2.1884130
C	-2.6136300	1.4309800	-0.7672170
O	-5.5195680	1.2971230	2.3202550
C	-3.2500450	-1.5973350	-1.0414220
C	-1.8125020	-1.5611060	-0.5659500
O	-0.9236720	-1.5623600	-1.5469910
O	-1.5061390	-1.5761440	0.6452320
H	-5.2302090	-0.8750720	-0.8301710
H	-4.9966290	-1.2824530	1.5375580
H	-3.3815950	-0.5533860	1.5923340
H	-5.7616810	0.9780570	-2.1904670
H	-4.6153290	2.3289030	-2.3983250
H	-4.1903350	0.7080640	-3.0014220
H	-1.9970200	1.0064260	-1.5742780
H	-2.6148050	2.5249350	-0.8801270
H	-2.1460440	1.1915630	0.1995190
H	-3.6162760	-2.6094450	-0.7934240
H	-3.2521930	-1.5222460	-2.1388300
H	0.0360850	-1.5782610	-1.1657560
C	4.0552560	0.9164320	0.8444070
C	4.2408910	-0.5799550	0.4359960
O	4.8266510	1.6322390	-0.1889850
C	4.9724590	0.8694410	-1.3234370
C	4.3616490	-0.5047350	-1.0913510
C	4.6962730	1.2522730	2.1884060
C	2.6136320	1.4309870	0.7672070
O	5.5195720	1.2971070	-2.3202610
C	3.2500430	-1.5973290	1.0414310
C	1.8125000	-1.5611020	0.5659590
O	0.9236700	-1.5623510	1.5470000
O	1.5061370	-1.5761440	-0.6452230
H	5.2302080	-0.8750690	0.8301750

H	4.9966250	-1.2824630	-1.5375530
H	3.3815930	-0.5533910	-1.5923310
H	5.7616800	0.9780630	2.1904650
H	4.6153330	2.3289160	2.3983110
H	4.1903310	0.7080830	3.0014190
H	1.9970200	1.0064380	1.5742690
H	2.6148090	2.5249420	0.8801110
H	2.1460480	1.1915640	-0.1995290
H	3.6162730	-2.6094410	0.7934390
H	3.2521910	-1.5222320	2.1388390
H	-0.0360860	-1.5782550	1.1657650

***cis*-Pinic Acid -Terpenylic Acid non-covalent Dimer alkyl carboxylate– Gas Phase @ 298 K**

C	4.3921650	0.5538700	0.9680840
C	2.9632730	0.6016520	1.5196280
C	5.3875560	0.1047830	2.0342770
O	4.7581250	1.9343350	0.5942380
C	4.5513430	-0.2156820	-0.3812980
C	4.1749450	0.8452590	-1.4230180
C	4.5909230	2.1473070	-0.7531650
C	3.8984810	-1.6130250	-0.4820890
C	2.3871270	-1.7249570	-0.4543500
O	1.8057970	-2.4368920	0.3902220
O	1.7596460	-1.0589030	-1.4109260
O	4.7695860	3.2370840	-1.2598950
H	2.9182150	1.3355590	2.3375470
H	2.2387830	0.9103630	0.7506270
H	2.6581420	-0.3772920	1.9182600
H	5.1937160	-0.9402870	2.3225640
H	6.4194660	0.1824690	1.6607850
H	5.2976730	0.7285540	2.9357910
H	5.6354400	-0.4038310	-0.4874320
H	3.0924440	0.8757860	-1.6254390
H	4.6845140	0.7355560	-2.3901520
H	4.2215010	-2.0590160	-1.4391850
H	4.2788460	-2.2612970	0.3204100
H	0.7301360	-1.2012080	-1.3429030
C	-5.3739960	1.6970020	-0.3258070
C	-3.9399270	1.2553230	-0.2157820
C	-3.4866800	0.2946250	-1.3492720
C	-3.7403980	-0.9075040	-0.4054670
C	-3.7217130	0.0658530	0.8289770
C	-2.8924700	-2.1927910	-0.4513810
C	-1.3895720	-2.0413690	-0.4430370
C	-2.3525530	0.2283530	1.5011350
C	-4.8037750	-0.1782670	1.8817710

O	-6.2596560	1.1410830	-0.9649640
O	-5.6173890	2.8145770	0.4266780
O	-0.7745680	-2.7345900	0.5038210
O	-0.7856620	-1.3466890	-1.2908660
H	-3.3070220	2.1332180	-0.0194890
H	-2.4247510	0.4302250	-1.5922460
H	-4.0837820	0.3234070	-2.2714840
H	-4.7855940	-1.2314720	-0.5437600
H	-3.1793390	-2.8654320	0.3709850
H	-3.1311980	-2.7148110	-1.3955780
H	-1.5531210	0.4419880	0.7747230
H	-2.3831580	1.0662650	2.2165130
H	-2.0758580	-0.6793840	2.0615250
H	-4.5881460	-1.1063380	2.4373160
H	-4.8437150	0.6453630	2.6132180
H	-5.8010100	-0.2847010	1.4269500
H	-6.5742050	3.0062240	0.3232010
H	0.2466380	-2.6125480	0.4355520

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer alkyl carboxylate– Gas Phase @ 373 K**

C	4.3921650	0.5538700	0.9680840
C	2.9632730	0.6016520	1.5196280
C	5.3875560	0.1047830	2.0342770
O	4.7581250	1.9343350	0.5942380
C	4.5513430	-0.2156820	-0.3812980
C	4.1749450	0.8452590	-1.4230180
C	4.5909230	2.1473070	-0.7531650
C	3.8984810	-1.6130250	-0.4820890
C	2.3871270	-1.7249570	-0.4543500
O	1.8057970	-2.4368920	0.3902220
O	1.7596460	-1.0589030	-1.4109260
O	4.7695860	3.2370840	-1.2598950
H	2.9182150	1.3355590	2.3375470
H	2.2387830	0.9103630	0.7506270
H	2.6581420	-0.3772920	1.9182600
H	5.1937160	-0.9402870	2.3225640
H	6.4194660	0.1824690	1.6607850
H	5.2976730	0.7285540	2.9357910
H	5.6354400	-0.4038310	-0.4874320
H	3.0924440	0.8757860	-1.6254390
H	4.6845140	0.7355560	-2.3901520
H	4.2215010	-2.0590160	-1.4391850
H	4.2788460	-2.2612970	0.3204100
H	0.7301360	-1.2012080	-1.3429030
C	-5.3739960	1.6970020	-0.3258070
C	-3.9399270	1.2553230	-0.2157820

C	-3.4866800	0.2946250	-1.3492720
C	-3.7403980	-0.9075040	-0.4054670
C	-3.7217130	0.0658530	0.8289770
C	-2.8924700	-2.1927910	-0.4513810
C	-1.3895720	-2.0413690	-0.4430370
C	-2.3525530	0.2283530	1.5011350
C	-4.8037750	-0.1782670	1.8817710
O	-6.2596560	1.1410830	-0.9649640
O	-5.6173890	2.8145770	0.4266780
O	-0.7745680	-2.7345900	0.5038210
O	-0.7856620	-1.3466890	-1.2908660
H	-3.3070220	2.1332180	-0.0194890
H	-2.4247510	0.4302250	-1.5922460
H	-4.0837820	0.3234070	-2.2714840
H	-4.7855940	-1.2314720	-0.5437600
H	-3.1793390	-2.8654320	0.3709850
H	-3.1311980	-2.7148110	-1.3955780
H	-1.5531210	0.4419880	0.7747230
H	-2.3831580	1.0662650	2.2165130
H	-2.0758580	-0.6793840	2.0615250
H	-4.5881460	-1.1063380	2.4373160
H	-4.8437150	0.6453630	2.6132180
H	-5.8010100	-0.2847010	1.4269500
H	-6.5742050	3.0062240	0.3232010
H	0.2466380	-2.6125480	0.4355520

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer carboxylate– Gas Phase @ 298 K**

C	-1.3928490	-1.3791750	-0.4241850
C	-2.8792510	-1.3036270	-0.2360460
C	-3.6410720	-0.4899850	-1.3174920
C	-3.6594090	0.7337080	-0.3665280
C	-3.3268970	-0.2111410	0.8454500
C	-4.8342860	1.7257800	-0.3238110
C	-6.2300280	1.1417660	-0.2641740
C	-4.5499060	-0.7303500	1.6110650
C	-2.2719530	0.3104140	1.8224460
O	-0.7598220	-0.5666800	-1.1376580
O	-0.8118250	-2.3543520	0.2617190
O	-6.9911060	1.7383400	0.7041090
O	-6.6832410	0.2721770	-0.9971940
H	-3.2521630	-2.3136910	-0.0124440
H	-4.6432320	-0.9004880	-1.4969410
H	-3.1191920	-0.3545020	-2.2751090
H	-2.7573230	1.3368170	-0.5643490
H	-4.7037460	2.4350140	0.5079220
H	-4.8082410	2.3217260	-1.2542110

H	-5.3140140	-1.1533560	0.9416550
H	-4.2444680	-1.5218790	2.3145490
H	-5.0166560	0.0766010	2.1996390
H	-2.6862670	1.1430030	2.4152740
H	-1.9549200	-0.4748500	2.5279230
H	-1.3783020	0.6871860	1.3003500
H	0.2088010	-2.3265660	0.1338290
H	-7.8816650	1.3309910	0.6362230
C	4.7737420	0.1741670	0.9163120
C	3.4100460	0.2556550	1.6101820
C	5.7808360	-0.6088420	1.7541350
O	5.2875720	1.5541150	0.8077920
C	4.7268780	-0.2883520	-0.5745340
C	4.4158460	1.0135020	-1.3235910
C	5.0483070	2.0788090	-0.4395160
C	3.8885040	-1.5450780	-0.9003160
C	2.3816440	-1.4902350	-0.7401500
O	1.7782620	-2.3088170	-0.0164550
O	1.7768820	-0.5558420	-1.4559800
O	5.3294900	3.2274080	-0.7195540
H	3.5245690	0.7864640	2.5666390
H	2.6759560	0.8083070	1.0043460
H	3.0099640	-0.7477120	1.8188630
H	5.4745420	-1.6637670	1.8326910
H	6.7822480	-0.5647530	1.3006670
H	5.8429290	-0.1959380	2.7717730
H	5.7653840	-0.5687980	-0.8292340
H	3.3344610	1.2084760	-1.4029910
H	4.8321820	1.0658440	-2.3389810
H	4.0751260	-1.8004130	-1.9583140
H	4.2401840	-2.3946210	-0.2973170
H	0.7432440	-0.5919870	-1.3121510

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer carboxylate– Gas Phase @ 373 K**

C	-1.3928490	-1.3791750	-0.4241850
C	-2.8792510	-1.3036270	-0.2360460
C	-3.6410720	-0.4899850	-1.3174920
C	-3.6594090	0.7337080	-0.3665280
C	-3.3268970	-0.2111410	0.8454500
C	-4.8342860	1.7257800	-0.3238110
C	-6.2300280	1.1417660	-0.2641740
C	-4.5499060	-0.7303500	1.6110650
C	-2.2719530	0.3104140	1.8224460
O	-0.7598220	-0.5666800	-1.1376580
O	-0.8118250	-2.3543520	0.2617190
O	-6.9911060	1.7383400	0.7041090

O	-6.6832410	0.2721770	-0.9971940
H	-3.2521630	-2.3136910	-0.0124440
H	-4.6432320	-0.9004880	-1.4969410
H	-3.1191920	-0.3545020	-2.2751090
H	-2.7573230	1.3368170	-0.5643490
H	-4.7037460	2.4350140	0.5079220
H	-4.8082410	2.3217260	-1.2542110
H	-5.3140140	-1.1533560	0.9416550
H	-4.2444680	-1.5218790	2.3145490
H	-5.0166560	0.0766010	2.1996390
H	-2.6862670	1.1430030	2.4152740
H	-1.9549200	-0.4748500	2.5279230
H	-1.3783020	0.6871860	1.3003500
H	0.2088010	-2.3265660	0.1338290
H	-7.8816650	1.3309910	0.6362230
C	4.7737420	0.1741670	0.9163120
C	3.4100460	0.2556550	1.6101820
C	5.7808360	-0.6088420	1.7541350
O	5.2875720	1.5541150	0.8077920
C	4.7268780	-0.2883520	-0.5745340
C	4.4158460	1.0135020	-1.3235910
C	5.0483070	2.0788090	-0.4395160
C	3.8885040	-1.5450780	-0.9003160
C	2.3816440	-1.4902350	-0.7401500
O	1.7782620	-2.3088170	-0.0164550
O	1.7768820	-0.5558420	-1.4559800
O	5.3294900	3.2274080	-0.7195540
H	3.5245690	0.7864640	2.5666390
H	2.6759560	0.8083070	1.0043460
H	3.0099640	-0.7477120	1.8188630
H	5.4745420	-1.6637670	1.8326910
H	6.7822480	-0.5647530	1.3006670
H	5.8429290	-0.1959380	2.7717730
H	5.7653840	-0.5687980	-0.8292340
H	3.3344610	1.2084760	-1.4029910
H	4.8321820	1.0658440	-2.3389810
H	4.0751260	-1.8004130	-1.9583140
H	4.2401840	-2.3946210	-0.2973170
H	0.7432440	-0.5919870	-1.3121510

**Cartesian coordinates for optimized monomers and dimers in the water solvent continuum
studied in the article**

Aldehyde/Ester Monomer 1 @ 298 K

O	-3.2129340	0.5744150	-0.9006070
C	-2.9834380	-0.7626400	-0.4788900
O	-2.0000960	-0.8920520	0.5283130
C	-0.6519270	-0.7184540	0.0938410
C	0.3947810	-1.3491830	1.0248130
C	1.3153800	-0.1169280	0.8031150
C	0.0465990	0.6821350	0.2448690
C	0.2072570	1.4971760	-1.0364820
C	-0.5547580	1.5330920	1.3671370
C	2.3874020	-0.3357860	-0.2277400
O	2.3821210	-1.1837510	-1.1126970
O	3.4041130	0.5725550	-0.1023890
H	-3.6291050	1.0532820	-0.1603490
H	-3.8936370	-1.2110060	-0.0468400
H	-2.6812110	-1.3008790	-1.3945070
H	-0.5463610	-1.0843840	-0.9444120
H	0.7973380	-2.3277170	0.7303530
H	0.0278610	-1.3915790	2.0603000
H	1.7603730	0.3400860	1.6986120
H	0.6640570	0.9032840	-1.8438620
H	-0.7841940	1.8280340	-1.3851650
H	0.8325920	2.3894250	-0.8688590
H	0.1167270	2.3743450	1.6037400
H	-1.5240560	1.9493000	1.0518790
H	-0.7229190	0.9536030	2.2876530
H	4.0291250	0.3783930	-0.8334750

Norpinic Acid @ 298 K

C	-1.0626320	-0.2642760	-0.7805040
C	-0.0006910	-1.3859390	-0.6243580
C	0.8070230	-0.4983030	0.3443420
C	-0.0140150	0.7647740	-0.1605810
C	0.6885590	1.5299030	-1.2877040
C	-0.4975390	1.7210720	0.9283920
H	-1.3782680	-0.0085640	-1.8021980
H	0.5563530	-1.5637360	-1.5544830
H	-0.3633020	-2.3382150	-0.2159560
H	0.5356680	-0.7120990	1.3923990
H	-0.9941510	1.1896030	1.7548880
H	0.3539980	2.2855980	1.3452540
H	-1.2060440	2.4584270	0.5170810

H	-0.0114020	2.2470220	-1.7455760
H	1.5503300	2.0970640	-0.8995340
H	1.0601390	0.8587350	-2.0762390
C	2.3114360	-0.4531800	0.1782010
O	2.9211150	-0.8935550	-0.7787120
O	3.0004720	0.1903990	1.1796490
C	-2.2782530	-0.4619140	0.0854950
O	-3.3574120	0.2325550	-0.3862360
O	-2.3293390	-1.1235040	1.1159520
H	2.3794590	0.4544870	1.8866170
H	-4.0848020	0.0717050	0.2528280

***cis*-Pinic Acid @ 298 K**

C	-2.6419900	-0.4665740	-0.1083180
C	-1.2797990	-0.3022900	-0.7244650
C	-0.2542160	-1.3861450	-0.2923470
C	0.3131210	-0.4043200	0.7639820
C	-0.3783820	0.7918800	0.0135000
C	1.8036030	-0.3731210	1.1441260
C	2.8059670	-0.3711330	0.0095480
C	0.5070710	1.5002780	-1.0190210
C	-1.0767550	1.8179230	0.9072740
O	-2.9126580	-1.1043080	0.9027430
O	-3.5970960	0.2332040	-0.7974170
O	3.7605510	0.5965640	0.1732640
O	2.8289640	-1.1452540	-0.9386540
H	-1.3925600	-0.1213680	-1.8035320
H	0.4626780	-1.6062780	-1.0940860
H	-0.6801290	-2.3228460	0.0938230
H	-0.2399950	-0.5578510	1.7058570
H	2.0091020	0.4801190	1.8087070
H	2.0237100	-1.2873530	1.7247920
H	0.9962150	0.7934230	-1.7061990
H	-0.1020130	2.1903430	-1.6255280
H	1.2909950	2.0964110	-0.5233250
H	-0.3273030	2.4122980	1.4565670
H	-1.6857660	2.5185310	0.3127610
H	-1.7312000	1.3360840	1.6504290
H	-4.4357660	0.0972110	-0.3064540
H	4.3822190	0.4906420	-0.5789820

***cis*-Pinic Acid @ 373 K**

C	-2.6419900	-0.4665740	-0.1083180
C	-1.2797990	-0.3022900	-0.7244650
C	-0.2542160	-1.3861450	-0.2923470

C	0.3131210	-0.4043200	0.7639820
C	-0.3783820	0.7918800	0.0135000
C	1.8036030	-0.3731210	1.1441260
C	2.8059670	-0.3711330	0.0095480
C	0.5070710	1.5002780	-1.0190210
C	-1.0767550	1.8179230	0.9072740
O	-2.9126580	-1.1043080	0.9027430
O	-3.5970960	0.2332040	-0.7974170
O	3.7605510	0.5965640	0.1732640
O	2.8289640	-1.1452540	-0.9386540
H	-1.3925600	-0.1213680	-1.8035320
H	0.4626780	-1.6062780	-1.0940860
H	-0.6801290	-2.3228460	0.0938230
H	-0.2399950	-0.5578510	1.7058570
H	2.0091020	0.4801190	1.8087070
H	2.0237100	-1.2873530	1.7247920
H	0.9962150	0.7934230	-1.7061990
H	-0.1020130	2.1903430	-1.6255280
H	1.2909950	2.0964110	-0.5233250
H	-0.3273030	2.4122980	1.4565670
H	-1.6857660	2.5185310	0.3127610
H	-1.7312000	1.3360840	1.6504290
H	-4.4357660	0.0972110	-0.3064540
H	4.3822190	0.4906420	-0.5789820

Pinonaldehyde @ 298 K

C	-2.3756330	0.5604230	-0.5591350
C	-2.6156640	-0.9212570	-0.3757890
O	2.8843950	-0.2103820	-1.1378510
C	2.1461090	-0.6719690	-0.2680550
C	2.6969070	-1.4611470	0.9057280
C	0.6452040	-0.4542350	-0.3021050
C	0.0104180	0.1204780	-1.5862610
C	-0.9111890	1.0278770	-0.7183200
C	0.0631970	0.7966150	0.5019160
C	-0.5348400	0.5072960	1.8781560
C	1.0685760	1.9540890	0.5928020
O	-3.2663600	-1.4131830	0.5377810
H	-2.8789410	1.0976770	0.2602300
H	-2.8988610	0.8229190	-1.5007440
H	-2.1872020	-1.5852170	-1.1702530
H	3.7926660	-1.4050970	0.9215580
H	2.2827780	-1.0927640	1.8587800
H	2.3879870	-2.5168680	0.8178940
H	0.1349850	-1.3676430	0.0523310
H	-0.4671810	-0.5953550	-2.2720240

H	0.7543910	0.6967920	-2.1548780
H	-0.9447290	2.0837920	-1.0369510
H	-1.2589530	-0.3198340	1.8669400
H	0.2608620	0.2494700	2.5971050
H	-1.0494020	1.3994630	2.2733650
H	0.5524820	2.8677270	0.9311340
H	1.8700530	1.7350340	1.3174970
H	1.5462680	2.1693900	-0.3750450

Pinonaldehyde @ 373 K

C	-2.3756330	0.5604230	-0.5591350
C	-2.6156640	-0.9212570	-0.3757890
O	2.8843950	-0.2103820	-1.1378510
C	2.1461090	-0.6719690	-0.2680550
C	2.6969070	-1.4611470	0.9057280
C	0.6452040	-0.4542350	-0.3021050
C	0.0104180	0.1204780	-1.5862610
C	-0.9111890	1.0278770	-0.7183200
C	0.0631970	0.7966150	0.5019160
C	-0.5348400	0.5072960	1.8781560
C	1.0685760	1.9540890	0.5928020
O	-3.2663600	-1.4131830	0.5377810
H	-2.8789410	1.0976770	0.2602300
H	-2.8988610	0.8229190	-1.5007440
H	-2.1872020	-1.5852170	-1.1702530
H	3.7926660	-1.4050970	0.9215580
H	2.2827780	-1.0927640	1.8587800
H	2.3879870	-2.5168680	0.8178940
H	0.1349850	-1.3676430	0.0523310
H	-0.4671810	-0.5953550	-2.2720240
H	0.7543910	0.6967920	-2.1548780
H	-0.9447290	2.0837920	-1.0369510
H	-1.2589530	-0.3198340	1.8669400
H	0.2608620	0.2494700	2.5971050
H	-1.0494020	1.3994630	2.2733650
H	0.5524820	2.8677270	0.9311340
H	1.8700530	1.7350340	1.3174970
H	1.5462680	2.1693900	-0.3750450

***cis*-Pinonic Acid @ 298 K**

C	-2.8637540	-0.1807250	-0.3946580
C	-1.8717840	-0.9063950	0.4774570
C	-0.4133290	-0.7424640	0.0582300
C	0.6512600	-1.4615720	0.9223940
C	1.5946620	-0.2410290	0.7889500

C	0.3341870	0.6234740	0.2884580
C	0.5073110	1.5059300	-0.9478730
C	-0.2218410	1.4454510	1.4547740
O	-2.7087590	0.1051930	-1.5842520
O	-4.0172980	0.1154870	0.2707390
H	-4.6321030	0.5443640	-0.3660150
H	-2.0332990	-0.6144280	1.5262430
H	-2.1440070	-1.9775440	0.4158620
H	-0.3001950	-1.0344170	-0.9985090
H	1.0341940	-2.4181930	0.5379630
H	0.3213990	-1.5954180	1.9635960
H	2.0260210	0.1551930	1.7217480
H	-0.3428110	0.8433270	2.3690480
H	0.4579370	2.2811930	1.6877190
H	-1.2051780	1.8720130	1.1932750
H	-0.4683970	1.9244890	-1.2445060
H	1.1854030	2.3519360	-0.7476890
H	0.9016370	0.9411630	-1.8076690
C	2.6913870	-0.3551520	-0.2361310
O	2.6989310	-1.2462760	-1.1062800
C	3.7913530	0.6719460	-0.1663780
H	4.3930010	0.6736840	-1.0848460
H	3.3835740	1.6756720	0.0304320
H	4.4431220	0.4249460	0.6903520

***cis*-Pinonic Acid @ 373 K**

C	-2.8637540	-0.1807250	-0.3946580
C	-1.8717840	-0.9063950	0.4774570
C	-0.4133290	-0.7424640	0.0582300
C	0.6512600	-1.4615720	0.9223940
C	1.5946620	-0.2410290	0.7889500
C	0.3341870	0.6234740	0.2884580
C	0.5073110	1.5059300	-0.9478730
C	-0.2218410	1.4454510	1.4547740
O	-2.7087590	0.1051930	-1.5842520
O	-4.0172980	0.1154870	0.2707390
H	-4.6321030	0.5443640	-0.3660150
H	-2.0332990	-0.6144280	1.5262430
H	-2.1440070	-1.9775440	0.4158620
H	-0.3001950	-1.0344160	-0.9985090
H	1.0341940	-2.4181930	0.5379630
H	0.3213990	-1.5954180	1.9635960
H	2.0260210	0.1551930	1.7217480
H	-0.3428110	0.8433270	2.3690480
H	0.4579370	2.2811930	1.6877190

H	-1.2051780	1.8720130	1.1932760
H	-0.4683970	1.9244890	-1.2445050
H	1.1854030	2.3519360	-0.7476890
H	0.9016370	0.9411630	-1.8076690
C	2.6913870	-0.3551520	-0.2361310
O	2.6989310	-1.2462760	-1.1062800
C	3.7913530	0.6719460	-0.1663780
H	4.3930010	0.6736840	-1.0848460
H	3.3835740	1.6756720	0.0304320
H	4.4431220	0.4249460	0.6903520

Hemi-acetal Monomer 1 @ 298 K

O	-2.1698640	-1.6429390	0.2243940
C	-2.9252680	-0.7118040	0.0201360
C	-2.5394260	0.6905890	-0.4442290
C	-1.0630810	0.9952640	-0.7364140
C	-0.2326230	-0.0617770	-1.5226280
C	0.6195640	-0.3502590	-0.2645130
C	0.0019000	0.9531530	0.4286490
C	0.9212050	2.1793210	0.3446920
C	-0.4842210	0.7533240	1.8639490
C	2.1128500	-0.3964630	-0.4053350
O	2.7243830	0.0928580	-1.3620770
O	-4.2725340	-0.8987980	0.2085460
C	2.9229500	-1.0502140	0.7075890
O	4.3073290	-0.9111140	0.4942290
H	-2.9232110	1.4082200	0.3060310
H	-3.1191680	0.8892570	-1.3661510
H	-1.0629920	1.9851230	-1.2245910
H	0.3688630	0.3868580	-2.3261630
H	-0.7811260	-0.9280400	-1.9167200
H	0.2582100	-1.2395520	0.2742990
H	1.3214620	2.3270730	-0.6700360
H	0.3596030	3.0855720	0.6272220
H	1.7786630	2.0899860	1.0320020
H	0.3756850	0.6283210	2.5433110
H	-1.0446640	1.6364680	2.2163360
H	-1.1224980	-0.1351210	1.9692450
H	-4.7604050	-0.0757390	0.0094430
H	2.6269190	-0.6011730	1.6780650
H	2.6309420	-2.1203160	0.7577700
H	4.3761000	-0.4638050	-0.3821660

Hydroperoxide Monomer @ 298 K

C	-2.2637990	-1.0850850	-0.3639830
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C	-0.9154160	-0.4259710	-0.2121700
C	-0.0393440	-0.6326800	1.0496440
C	0.3436500	0.8793410	1.0191470
C	-0.8273980	1.1408810	-0.0150320
C	-0.5226840	1.9622510	-1.2664680
C	-2.0499520	1.7196030	0.7102780
C	1.7795760	1.2542290	0.6130820
C	2.5029130	0.3891400	-0.4265850
O	3.1404880	-0.6809970	0.3130220
O	3.8750290	-1.5194350	-0.6512440
C	-2.5946160	-2.2625430	0.5108280
O	-3.0759090	-0.6615490	-1.2096800
H	-0.3535530	-0.7022390	-1.1235740
H	0.7862020	-1.3520710	0.9524040
H	-0.6275220	-0.8930720	1.9416590
H	0.1400460	1.3931370	1.9734250
H	0.3425490	1.5733200	-1.8251150
H	-1.3903950	1.9533730	-1.9469660
H	-0.3150690	3.0142570	-1.0065580
H	-1.8290410	2.7450420	1.0508360
H	-2.9305080	1.7656090	0.0494220
H	-2.3207940	1.1228120	1.5971790
H	1.7858420	2.2910960	0.2365510
H	2.4137760	1.2711100	1.5174540
H	1.8247960	-0.0484530	-1.1781250
H	3.2839340	0.9708780	-0.9443810
H	3.1967400	-2.1949260	-0.8759030
H	-3.5111100	-2.7598460	0.1675950
H	-1.7541320	-2.9752000	0.5360860
H	-2.7362160	-1.9139790	1.5487670

Hydroperoxide Monomer @ 373 K

C	-2.2637990	-1.0850850	-0.3639830
C	-0.9154160	-0.4259710	-0.2121700
C	-0.0393440	-0.6326800	1.0496440
C	0.3436500	0.8793410	1.0191470
C	-0.8273980	1.1408810	-0.0150320
C	-0.5226840	1.9622510	-1.2664680
C	-2.0499520	1.7196030	0.7102780
C	1.7795760	1.2542290	0.6130820
C	2.5029130	0.3891400	-0.4265850
O	3.1404880	-0.6809970	0.3130220
O	3.8750290	-1.5194350	-0.6512440
C	-2.5946160	-2.2625430	0.5108280
O	-3.0759090	-0.6615490	-1.2096800
H	-0.3535530	-0.7022390	-1.1235740

H	0.7862020	-1.3520710	0.9524040
H	-0.6275220	-0.8930720	1.9416590
H	0.1400460	1.3931370	1.9734250
H	0.3425490	1.5733200	-1.8251150
H	-1.3903950	1.9533730	-1.9469660
H	-0.3150690	3.0142570	-1.0065580
H	-1.8290410	2.7450420	1.0508360
H	-2.9305080	1.7656090	0.0494220
H	-2.3207940	1.1228120	1.5971790
H	1.7858420	2.2910960	0.2365510
H	2.4137760	1.2711100	1.5174540
H	1.8247960	-0.0484530	-1.1781250
H	3.2839340	0.9708780	-0.9443810
H	3.1967400	-2.1949260	-0.8759030
H	-3.5111100	-2.7598460	0.1675950
H	-1.7541320	-2.9752000	0.5360860
H	-2.7362160	-1.9139790	1.5487670

2,2-dimethyl-3-formyl-cyclobutyl-methanoic acid @ 298 K

C	2.3789130	0.0837110	-0.0418070
C	1.0692420	-0.0916760	0.7253960
C	0.2123660	-1.3238700	0.3010720
C	-0.7582830	-0.3793590	-0.4387440
C	-0.1403880	0.8514920	0.3543680
C	-0.9398370	1.2024420	1.6171180
C	0.1214580	2.1072840	-0.4765290
C	-2.2330420	-0.6278840	-0.2946360
O	-2.7638890	-1.4319250	0.4611950
O	-2.9673700	0.2001850	-1.1041540
H	1.3368530	-0.0508450	1.7938980
H	-0.2742110	-1.8187070	1.1530550
H	0.7017380	-2.0831200	-0.3268500
H	-0.5034400	-0.2793020	-1.5042610
H	-3.9079620	-0.0091470	-0.9192810
H	-1.1739870	0.3132470	2.2230020
H	-0.3604430	1.8985790	2.2455960
H	-1.8910010	1.6957210	1.3580780
H	-0.8359960	2.5528100	-0.7923870
H	0.6608680	2.8662250	0.1154480
H	0.7097170	1.8823220	-1.3776900
O	3.4003330	-0.7841410	0.4379690
O	2.1359230	-0.1401380	-1.4305240
H	3.0473300	-1.6950040	0.4036660
H	2.9937850	-0.0527040	-1.8859590
H	2.7942060	1.0952300	0.1203700

Terpenylic Acid @ 298 K

C	0.7171420	1.0133160	-0.0804370
C	-0.0124620	1.0985130	-1.4245980
C	0.9440600	2.3970700	0.5216160
O	2.0514830	0.4381630	-0.3472780
C	0.1096990	-0.0047540	0.9357470
C	0.7333840	-1.3350200	0.4963780
C	2.0758300	-0.9092790	-0.0829440
C	-1.4163440	0.0522760	1.1748120
C	-2.3626800	-0.3117450	0.0465790
O	-3.2180740	0.4244250	-0.4221200
O	-2.2057060	-1.6037650	-0.3776780
O	3.0566610	-1.5924480	-0.3014840
H	0.6084780	1.6636550	-2.1349530
H	-0.1920240	0.1018320	-1.8559160
H	-0.9781240	1.6151460	-1.3229540
H	-0.0188050	2.8621010	0.7850180
H	1.5644170	2.3308940	1.4278170
H	1.4526350	3.0541550	-0.1990640
H	0.5556220	0.2532890	1.9138270
H	0.1495480	-1.8400080	-0.2898810
H	0.8822800	-2.0597070	1.3085900
H	-1.6453040	-0.6340110	2.0087060
H	-1.7031550	1.0628010	1.4994620
H	-2.8822470	-1.7433900	-1.0750840

Terpenylic Acid @ 373 K

C	0.7171420	1.0133160	-0.0804370
C	-0.0124620	1.0985130	-1.4245980
C	0.9440600	2.3970700	0.5216160
O	2.0514830	0.4381630	-0.3472780
C	0.1096990	-0.0047540	0.9357470
C	0.7333840	-1.3350200	0.4963780
C	2.0758300	-0.9092790	-0.0829440
C	-1.4163440	0.0522760	1.1748120
C	-2.3626800	-0.3117450	0.0465790
O	-3.2180740	0.4244250	-0.4221200
O	-2.2057060	-1.6037650	-0.3776780
O	3.0566610	-1.5924480	-0.3014840
H	0.6084780	1.6636550	-2.1349530
H	-0.1920240	0.1018320	-1.8559160
H	-0.9781240	1.6151460	-1.3229540
H	-0.0188050	2.8621010	0.7850180
H	1.5644170	2.3308940	1.4278170

H	1.4526350	3.0541550	-0.1990640
H	0.5556220	0.2532890	1.9138270
H	0.1495480	-1.8400080	-0.2898810
H	0.8822800	-2.0597070	1.3085900
H	-1.6453040	-0.6340110	2.0087060
H	-1.7031550	1.0628010	1.4994620
H	-2.8822470	-1.7433900	-1.0750840

Anhydride Dimer @ 298 K

C	-5.3339700	1.6083580	0.4465470
O	-4.8430120	2.8312700	-0.0702950
O	-4.9743690	0.4783180	-0.3346830
C	-3.5825320	0.1625870	-0.3149910
C	-3.1571510	-0.8135460	-1.4211280
C	-2.2585200	-1.5731620	-0.3991100
C	-3.0515630	-0.8369310	0.7800460
C	-0.7796470	-1.3050070	-0.4296230
O	0.0782080	-2.0830090	-0.0450720
O	-0.4963570	-0.0528730	-0.9647120
C	0.7849250	0.5614030	-0.9423040
O	1.0091060	1.3458280	-1.8400880
C	1.7041220	0.2621360	0.2054360
C	2.6336910	1.4634270	0.5584410
C	3.7976530	0.7973020	-0.2055510
C	3.0073480	-0.5751670	-0.2035480
C	-2.2294680	-0.2385920	1.9226090
C	-4.1436990	-1.7665080	1.3187030
C	3.3961060	-1.5021420	0.9529660
C	3.0140380	-1.3272680	-1.5314690
C	5.2002080	0.7676770	0.3383580
O	5.3238180	1.3727950	1.5599820
O	6.1509360	0.2368540	-0.2224330
H	-4.9206330	1.5459680	1.4679210
H	-6.4363010	1.5834620	0.4781820
H	-5.2483360	2.9685470	-0.9469890
H	-2.9856520	1.0899990	-0.3297390
H	-2.6669740	-0.3872240	-2.3059430
H	-4.0027030	-1.4428810	-1.7344490
H	-2.3688790	-2.6663500	-0.3728270
H	1.1542120	-0.1886550	1.0403390
H	2.8150210	1.5193540	1.6398840
H	2.3144120	2.4462950	0.1874740
H	3.8604570	1.1658740	-1.2411510
H	-1.4911490	0.4931620	1.5590150
H	-2.8882110	0.2847990	2.6348060

H	-1.6931130	-1.0231000	2.4817750
H	-3.6908320	-2.5848990	1.9013940
H	-4.8310000	-1.2157010	1.9803050
H	-4.7481520	-2.2073490	0.5120240
H	3.4300550	-0.9710520	1.9177900
H	2.6613490	-2.3173890	1.0344980
H	4.3888210	-1.9444520	0.7716160
H	4.0360200	-1.6810420	-1.7422730
H	2.3442550	-2.1998470	-1.4879990
H	2.7035840	-0.6844890	-2.3694220
H	6.2678560	1.2760870	1.8098910

***cis*-Pinic Acid Dimer @ 298 K**

O	6.2006380	-1.6981730	-0.5031050
C	6.9472640	-0.8432060	-0.0676810
C	6.5466400	0.4166040	0.6962070
C	5.0569740	0.6908970	0.9461590
C	4.1473370	-0.4946770	1.3911060
C	3.4007140	-0.4342300	0.0414300
C	4.0882200	0.9647270	-0.2725260
C	3.1802340	2.1641440	0.0350000
C	4.6805520	1.0993240	-1.6749390
C	1.8994730	-0.4686890	0.0434790
O	8.3019800	-0.9928510	-0.2458730
O	1.2240700	-0.4446610	1.0953420
O	1.3652670	-0.4921310	-1.1715950
H	6.9973970	1.2834640	0.1761050
H	7.0565480	0.3621930	1.6775070
H	5.0337230	1.5342200	1.6578570
H	3.4948250	-0.2341630	2.2364390
H	4.6480990	-1.4490240	1.6024410
H	3.7745840	-1.1863250	-0.6681230
H	2.7169290	2.0860900	1.0315360
H	3.7669890	3.0976580	0.0071880
H	2.3724970	2.2518740	-0.7096610
H	3.8692740	1.1430980	-2.4195270
H	5.2662760	2.0301540	-1.7699230
H	5.3242330	0.2484210	-1.9392740
H	8.7796350	-0.2365610	0.1476590
H	0.3340850	-0.4777630	-1.1143880
O	-6.2006520	-1.6981620	0.5031010
C	-6.9472720	-0.8431950	0.0676690
C	-6.5466360	0.4166190	-0.6962090
C	-5.0569670	0.6909010	-0.9461550
C	-4.1473370	-0.4946790	-1.3911040
C	-3.4007140	-0.4342420	-0.0414280

C	-4.0882150	0.9647170	0.2725350
C	-3.1802220	2.1641330	-0.0349770
C	-4.6805480	1.0993050	1.6749490
C	-1.8994730	-0.4687020	-0.0434780
O	-8.3019910	-0.9928400	0.2458400
O	-1.2240710	-0.4446430	-1.0953410
O	-1.3652670	-0.4921780	1.1715940
H	-6.9973870	1.2834770	-0.1760970
H	-7.0565440	0.3622230	-1.6775090
H	-5.0337060	1.5342270	-1.6578480
H	-3.4948240	-0.2341670	-2.2364360
H	-4.6481070	-1.4490200	-1.6024410
H	-3.7745850	-1.1863380	0.6681230
H	-2.7169150	2.0860860	-1.0315120
H	-3.7669750	3.0976490	-0.0071600
H	-2.3724880	2.2518550	0.7096870
H	-3.8692710	1.1430720	2.4195380
H	-5.2662710	2.0301360	1.7699380
H	-5.3242320	0.2484010	1.9392750
H	-8.7796390	-0.2365500	-0.1476990
H	-0.3340850	-0.4778000	1.1143870

***cis*-Pinic Acid Dimer @ 373 K**

O	6.2006380	-1.6981730	-0.5031050
C	6.9472640	-0.8432060	-0.0676810
C	6.5466400	0.4166040	0.6962070
C	5.0569740	0.6908970	0.9461590
C	4.1473370	-0.4946770	1.3911060
C	3.4007140	-0.4342300	0.0414300
C	4.0882200	0.9647270	-0.2725260
C	3.1802340	2.1641440	0.0350000
C	4.6805520	1.0993240	-1.6749390
C	1.8994730	-0.4686890	0.0434790
O	8.3019800	-0.9928510	-0.2458730
O	1.2240700	-0.4446610	1.0953420
O	1.3652670	-0.4921310	-1.1715950
H	6.9973970	1.2834640	0.1761050
H	7.0565480	0.3621930	1.6775070
H	5.0337230	1.5342200	1.6578570
H	3.4948250	-0.2341630	2.2364390
H	4.6480990	-1.4490240	1.6024410
H	3.7745840	-1.1863250	-0.6681230
H	2.7169290	2.0860900	1.0315360
H	3.7669890	3.0976580	0.0071880
H	2.3724970	2.2518740	-0.7096610
H	3.8692740	1.1430980	-2.4195270

H	5.2662760	2.0301540	-1.7699230
H	5.3242330	0.2484210	-1.9392740
H	8.7796350	-0.2365610	0.1476590
H	0.3340850	-0.4777630	-1.1143880
O	-6.2006520	-1.6981620	0.5031010
C	-6.9472720	-0.8431950	0.0676690
C	-6.5466360	0.4166190	-0.6962090
C	-5.0569670	0.6909010	-0.9461550
C	-4.1473370	-0.4946790	-1.3911040
C	-3.4007140	-0.4342420	-0.0414280
C	-4.0882150	0.9647170	0.2725350
C	-3.1802220	2.1641330	-0.0349770
C	-4.6805480	1.0993050	1.6749490
C	-1.8994730	-0.4687020	-0.0434780
O	-8.3019910	-0.9928400	0.2458400
O	-1.2240710	-0.4446430	-1.0953410
O	-1.3652670	-0.4921780	1.1715940
H	-6.9973870	1.2834770	-0.1760970
H	-7.0565440	0.3622230	-1.6775090
H	-5.0337060	1.5342270	-1.6578480
H	-3.4948240	-0.2341670	-2.2364360
H	-4.6481070	-1.4490200	-1.6024410
H	-3.7745850	-1.1863380	0.6681230
H	-2.7169150	2.0860860	-1.0315120
H	-3.7669750	3.0976490	-0.0071600
H	-2.3724880	2.2518550	0.7096870
H	-3.8692710	1.1430720	2.4195380
H	-5.2662710	2.0301360	1.7699380
H	-5.3242320	0.2484010	1.9392750
H	-8.7796390	-0.2365500	-0.1476990
H	-0.3340850	-0.4778000	1.1143870

Ester Dimer @ 298 K

O	4.0119160	1.2547320	-1.9899870
C	4.6714500	1.1059260	-0.9684760
C	4.5102840	0.0011170	0.0397380
C	3.8592280	-1.2880410	-0.5393860
C	2.5060140	-0.8447240	0.0310090
C	3.2298580	0.1782360	0.9799050
C	3.5241750	-0.4032660	2.3665180
C	2.6117620	1.5727350	1.0879610
O	5.6454120	1.9930940	-0.5972550
O	1.7524010	-1.9063210	0.6355970
C	0.3840280	-1.6928910	0.7094800
O	-0.1725560	-1.8739460	-0.6259950
C	-1.4959100	-1.6423030	-0.9005570

O	-1.8837280	-1.8182210	-2.0456170
C	-2.3905030	-1.1372990	0.2148470
C	-3.9038070	-1.3056410	-0.0899220
C	-3.9940110	0.1748800	-0.5077080
C	-2.5958730	0.4485690	0.1906060
C	-5.1698150	0.9765100	-0.0200180
O	-5.9955650	0.6172120	0.8088610
O	-5.2046600	2.2205710	-0.5920660
C	-2.7269800	0.9850540	1.6204230
C	-1.6265670	1.2988780	-0.6286490
H	5.4486920	-0.1248050	0.5980910
H	4.2308340	-2.1864310	-0.0264590
H	3.9140130	-1.4280430	-1.6268280
H	1.8945800	-0.3320780	-0.7291710
H	3.9657650	-1.4094270	2.3108640
H	4.2235250	0.2529200	2.9092050
H	2.5995730	-0.4823100	2.9602040
H	1.6846780	1.5343780	1.6844340
H	3.2976710	2.2738650	1.5913010
H	2.3610860	1.9873690	0.0991540
H	5.6561380	2.6873740	-1.2908350
H	-0.0207640	-2.4620860	1.3855450
H	0.1342800	-0.6767480	1.0683580
H	-2.0655420	-1.5176860	1.1952210
H	-4.4906520	-1.5061400	0.8172900
H	-4.1494590	-2.0385310	-0.8688460
H	-3.8858290	0.3067040	-1.5948590
H	-5.9795400	2.6776860	-0.2001900
H	-3.4490630	0.4073800	2.2176430
H	-1.7508450	0.9467790	2.1318650
H	-3.0580300	2.0363760	1.6127660
H	-2.0273920	2.3203900	-0.7302770
H	-0.6422530	1.3764820	-0.1367940
H	-1.4772280	0.8931650	-1.6406130

Aldol Addition Dimer @ 298 K

C	-5.0673440	1.6046360	0.0976840
C	-4.7658610	2.5233590	-1.0552560
O	-6.2060060	1.5800090	0.6061540
C	-3.9979860	0.6981970	0.6573730
C	-2.5142230	0.9475950	0.2670040
C	-2.5805550	-0.2444900	-0.7217360
C	-3.9165030	-0.7395270	-0.0541950
C	-3.7139000	-1.8167790	1.0176880
C	-5.0444740	-1.1324540	-1.0062580
C	-1.4182730	-1.1857480	-0.9298380

O	-1.6213020	-2.3681770	-1.2576080
C	-0.0061570	-0.6285920	-0.8376700
C	0.8670350	-1.1744210	0.3265080
O	0.1276830	-0.8840680	1.5462000
C	2.2453270	-0.4764370	0.2864730
C	3.2624020	-0.7137980	1.4346990
C	3.7990050	0.7334510	1.2319700
C	2.4985350	1.0793060	0.3990440
C	2.6762850	1.8162280	-0.9312430
C	1.5276030	1.8671240	1.2914170
C	5.1844580	0.9272530	0.5892110
C	5.5297950	0.1799960	-0.6760120
O	6.2046130	0.9679040	-1.5658160
O	5.3171020	-1.0120980	-0.9094810
H	-4.1267450	3.3484800	-0.6946380
H	-4.1976940	2.0116570	-1.8474870
H	-5.6941250	2.9435950	-1.4632240
H	-4.1924290	0.6024570	1.7364290
H	-1.8475540	0.7524610	1.1175530
H	-2.2679820	1.9293160	-0.1600970
H	-2.8076990	0.1326220	-1.7384470
H	-2.8825580	-1.5688730	1.6965350
H	-4.6304640	-1.9154640	1.6215010
H	-3.5000070	-2.7944520	0.5586240
H	-4.7991090	-2.0879170	-1.4979640
H	-5.9932660	-1.2687740	-0.4616210
H	-5.2046460	-0.3814060	-1.7959910
H	0.5057040	-0.8923230	-1.7775280
H	-0.0463630	0.4678380	-0.7680850
H	0.6783990	-1.1839050	2.2958030
H	2.7124450	-0.8053450	-0.6574500
H	3.9736040	-1.5413790	1.3035800
H	2.7833570	-0.8176440	2.4220690
H	3.8436700	1.3116840	2.1694990
H	3.3260010	1.2689620	-1.6324330
H	1.7014050	1.9506850	-1.4292270
H	3.1089620	2.8191320	-0.7754050
H	1.9326990	2.8809330	1.4551620
H	0.5338380	1.9747740	0.8283750
H	1.3921620	1.3972590	2.2772710
H	5.3678180	1.9984910	0.4201930
H	5.9436770	0.5936470	1.3216500
H	6.4551370	0.4045120	-2.3323410
C	1.0867360	-2.6934430	0.2411490
H	0.1326180	-3.2350200	0.3047930
H	1.5861640	-2.9733400	-0.6993840

H	1.7248360	-3.0199570	1.0786320
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Aldol Addition Dimer @ 373 K

C	-5.0673440	1.6046360	0.0976840
C	-4.7658610	2.5233590	-1.0552560
O	-6.2060060	1.5800090	0.6061540
C	-3.9979860	0.6981970	0.6573730
C	-2.5142230	0.9475950	0.2670040
C	-2.5805550	-0.2444900	-0.7217360
C	-3.9165030	-0.7395270	-0.0541950
C	-3.7139000	-1.8167790	1.0176880
C	-5.0444740	-1.1324540	-1.0062580
C	-1.4182730	-1.1857480	-0.9298380
O	-1.6213020	-2.3681770	-1.2576080
C	-0.0061570	-0.6285920	-0.8376700
C	0.8670350	-1.1744210	0.3265080
O	0.1276830	-0.8840680	1.5462000
C	2.2453270	-0.4764370	0.2864730
C	3.2624020	-0.7137980	1.4346990
C	3.7990050	0.7334510	1.2319700
C	2.4985350	1.0793060	0.3990440
C	2.6762850	1.8162280	-0.9312430
C	1.5276030	1.8671240	1.2914170
C	5.1844580	0.9272530	0.5892110
C	5.5297950	0.1799960	-0.6760120
O	6.2046130	0.9679040	-1.5658160
O	5.3171020	-1.0120980	-0.9094810
H	-4.1267450	3.3484800	-0.6946380
H	-4.1976940	2.0116570	-1.8474870
H	-5.6941250	2.9435950	-1.4632240
H	-4.1924290	0.6024570	1.7364290
H	-1.8475540	0.7524610	1.1175530
H	-2.2679820	1.9293160	-0.1600970
H	-2.8076990	0.1326220	-1.7384470
H	-2.8825580	-1.5688730	1.6965350
H	-4.6304640	-1.9154640	1.6215010
H	-3.5000070	-2.7944520	0.5586240
H	-4.7991090	-2.0879170	-1.4979640
H	-5.9932660	-1.2687740	-0.4616210
H	-5.2046460	-0.3814060	-1.7959910
H	0.5057040	-0.8923230	-1.7775280
H	-0.0463630	0.4678380	-0.7680850
H	0.6783990	-1.1839050	2.2958030
H	2.7124450	-0.8053450	-0.6574500
H	3.9736040	-1.5413790	1.3035800
H	2.7833570	-0.8176440	2.4220690

H	3.8436700	1.3116840	2.1694990
H	3.3260010	1.2689620	-1.6324330
H	1.7014050	1.9506850	-1.4292270
H	3.1089620	2.8191320	-0.7754050
H	1.9326990	2.8809330	1.4551620
H	0.5338380	1.9747740	0.8283750
H	1.3921620	1.3972590	2.2772710
H	5.3678180	1.9984910	0.4201930
H	5.9436770	0.5936470	1.3216500
H	6.4551370	0.4045120	-2.3323410
C	1.0867360	-2.6934430	0.2411490
H	0.1326180	-3.2350200	0.3047930
H	1.5861640	-2.9733400	-0.6993840
H	1.7248360	-3.0199570	1.0786320

Hemi-acetal Dimer @ 298 K

O	-7.2528280	1.5059950	-0.3497440
C	-6.4273960	0.4125430	-0.2754120
O	-6.6796210	-0.4635530	0.5312550
C	-5.2770500	0.3612670	-1.2783330
C	-3.8945600	-0.0593770	-0.7466930
C	-3.7091490	-1.2786050	0.1925940
C	-2.5834370	-0.5165960	0.9529650
C	-3.0861690	0.8391960	0.2609680
C	-2.0307190	1.7499370	-0.3698830
C	-3.9475450	1.6320990	1.2508900
C	-1.1345030	-0.8439740	0.6812990
C	-0.7691020	-1.7416630	-0.5100640
O	-0.2526360	-0.3765690	1.4088400
O	0.5489970	-1.5342160	-0.9800160
C	1.5496590	-2.4154330	-0.4485840
O	1.5466500	-2.4182240	0.9649930
C	2.8789360	-1.9922190	-1.0801470
C	3.3677400	-0.5706220	-0.7880210
C	4.5371410	-0.0494180	-1.6630060
C	5.1373270	0.6855220	-0.4399870
C	4.2022680	-0.2118650	0.5041880
C	3.4479400	0.4999710	1.6290310
C	5.0077140	-1.3869230	1.0689490
C	4.8332340	2.1701770	-0.3828230
O	3.9400750	2.6859890	-1.0566780
C	5.6881930	3.0033440	0.5575710
H	-6.9275390	2.1262670	-1.0300250
H	-5.1725160	1.3219170	-1.8139920
H	-5.5920120	-0.3775580	-2.0377860

H	-3.2638380	-0.1914040	-1.6440660
H	-3.4536050	-2.2370470	-0.2841960
H	-4.5822530	-1.4395630	0.8378920
H	-2.6908410	-0.4836350	2.0479360
H	-1.3970150	1.2193210	-1.0981090
H	-2.5192860	2.5855640	-0.8991080
H	-1.3665560	2.1805940	0.3958070
H	-3.3074940	2.0706110	2.0330090
H	-4.4654310	2.4657730	0.7466820
H	-4.7052700	1.0076080	1.7469300
H	-0.9420030	-2.7943040	-0.2019670
H	-1.4503680	-1.5352760	-1.3530350
H	1.3110850	-3.4577330	-0.7487180
H	1.2373650	-1.5212730	1.2450140
H	3.6348770	-2.7358020	-0.7766000
H	2.7618020	-2.0962010	-2.1744880
H	2.5220780	0.1314010	-0.8664220
H	4.2596250	0.5923870	-2.5117670
H	5.1952520	-0.8607390	-2.0131840
H	6.2119120	0.5280850	-0.2446160
H	2.8359510	1.3337750	1.2520750
H	2.7747160	-0.2039290	2.1423980
H	4.1424900	0.8935090	2.3908890
H	5.7148070	-1.0314610	1.8371650
H	4.3342200	-2.1231960	1.5368510
H	5.5939980	-1.9034750	0.2915650
H	5.2524930	4.0027370	0.6834310
H	5.8032470	2.5102750	1.5360490
H	6.7018950	3.1032280	0.1321770

Peroxyhemiacetal Dimer @ 298 K

C	-4.5947480	2.6447240	1.5748770
C	-4.9613480	1.2101490	1.3121230
O	-6.0354400	0.7336670	1.7294490
C	-4.0025590	0.3405860	0.5374190
C	-2.8383960	0.9335610	-0.2963680
C	-3.1310120	-0.1036190	-1.4249680
C	-4.5224100	-0.4312090	-0.7433250
C	-4.9067470	-1.8954480	-0.5385380
C	-5.6533980	0.3140680	-1.4648300
C	-2.1289340	-1.2533000	-1.6288730
C	-1.4075890	-1.8277480	-0.4013500
O	-0.2105140	-1.0349500	-0.2346090
O	0.4257120	-1.4781590	1.0381950
C	1.8175920	-1.9263500	0.7647380
O	2.2292260	-2.2638190	2.0787280

C	1.7782690	-3.2016680	-0.0582570
C	2.6291220	-0.7421530	0.2147480
C	2.6862880	-0.3995170	-1.2963830
C	4.1305230	0.1467980	-1.0891340
C	4.2090770	-0.6860610	0.2530490
C	4.8360440	-0.0366790	1.4890510
C	4.9228970	-2.0178680	-0.0277580
C	4.2974660	1.6796740	-1.0429640
C	3.2042770	2.4795490	-0.3308880
O	3.5293850	3.8650920	-0.5907820
O	2.4810280	4.6971940	0.0269130
H	-3.5571050	2.7203510	1.9387300
H	-4.6322680	3.2086030	0.6264230
H	-5.2882850	3.0990600	2.2943930
H	-3.6215200	-0.3980900	1.2660270
H	-1.8424590	0.8901830	0.1664920
H	-3.0288060	1.9660460	-0.6239260
H	-3.2817600	0.3654510	-2.4115720
H	-4.1235630	-2.4693390	-0.0195840
H	-5.8270600	-1.9647490	0.0650470
H	-5.1058980	-2.3877700	-1.5056110
H	-5.8151580	-0.1279470	-2.4621990
H	-6.6020910	0.2474620	-0.9080590
H	-5.4155890	1.3816140	-1.6058910
H	-2.6431430	-2.0899830	-2.1314160
H	-1.3496530	-0.9243620	-2.3394970
H	-2.0099510	-1.7675730	0.5198010
H	-1.1243000	-2.8808420	-0.5695810
H	2.4357890	-1.4360120	2.5597350
H	2.7906700	-3.5884750	-0.2313410
H	1.1945910	-3.9634210	0.4786940
H	1.3074440	-3.0146100	-1.0328620
H	2.2661930	0.1388080	0.7738120
H	1.9261710	0.2924260	-1.6872150
H	2.6884450	-1.3035940	-1.9232420
H	4.8573970	-0.2154790	-1.8351170
H	4.3388160	0.9032000	1.7718720
H	4.7742230	-0.7192650	2.3538480
H	5.9042520	0.1792580	1.3177770
H	6.0015680	-1.8269480	-0.1585200
H	4.8072870	-2.7285860	0.8063890
H	4.5630860	-2.5032430	-0.9481220
H	5.2742680	1.9209990	-0.5895370
H	4.3339740	2.0372660	-2.0870620
H	2.2043910	2.2661700	-0.7434700
H	3.1946860	2.3170320	0.7593970

H	2.8636890	4.8592370	0.9180310
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Peroxyhemiacetal Dimer @ 373 K

C	-4.5947480	2.6447240	1.5748770
C	-4.9613480	1.2101490	1.3121230
O	-6.0354400	0.7336670	1.7294490
C	-4.0025590	0.3405860	0.5374190
C	-2.8383960	0.9335610	-0.2963680
C	-3.1310120	-0.1036190	-1.4249680
C	-4.5224100	-0.4312090	-0.7433250
C	-4.9067470	-1.8954480	-0.5385380
C	-5.6533980	0.3140680	-1.4648300
C	-2.1289340	-1.2533000	-1.6288730
C	-1.4075890	-1.8277480	-0.4013500
O	-0.2105140	-1.0349500	-0.2346090
O	0.4257120	-1.4781590	1.0381950
C	1.8175920	-1.9263500	0.7647380
O	2.2292260	-2.2638190	2.0787280
C	1.7782690	-3.2016680	-0.0582570
C	2.6291220	-0.7421530	0.2147480
C	2.6862880	-0.3995170	-1.2963830
C	4.1305230	0.1467980	-1.0891340
C	4.2090770	-0.6860610	0.2530490
C	4.8360440	-0.0366790	1.4890510
C	4.9228970	-2.0178680	-0.0277580
C	4.2974660	1.6796740	-1.0429640
C	3.2042770	2.4795490	-0.3308880
O	3.5293850	3.8650920	-0.5907820
O	2.4810280	4.6971940	0.0269130
H	-3.5571050	2.7203510	1.9387300
H	-4.6322680	3.2086030	0.6264230
H	-5.2882850	3.0990600	2.2943930
H	-3.6215200	-0.3980900	1.2660270
H	-1.8424590	0.8901830	0.1664920
H	-3.0288060	1.9660460	-0.6239260
H	-3.2817600	0.3654510	-2.4115720
H	-4.1235630	-2.4693390	-0.0195840
H	-5.8270600	-1.9647490	0.0650470
H	-5.1058980	-2.3877700	-1.5056110
H	-5.8151580	-0.1279470	-2.4621990
H	-6.6020910	0.2474620	-0.9080590
H	-5.4155890	1.3816140	-1.6058910
H	-2.6431430	-2.0899830	-2.1314160
H	-1.3496530	-0.9243620	-2.3394970
H	-2.0099510	-1.7675730	0.5198010
H	-1.1243000	-2.8808420	-0.5695810

H	2.4357890	-1.4360120	2.5597350
H	2.7906700	-3.5884750	-0.2313410
H	1.1945910	-3.9634210	0.4786940
H	1.3074440	-3.0146100	-1.0328620
H	2.2661930	0.1388080	0.7738120
H	1.9261710	0.2924260	-1.6872150
H	2.6884450	-1.3035940	-1.9232420
H	4.8573970	-0.2154790	-1.8351170
H	4.3388160	0.9032000	1.7718720
H	4.7742230	-0.7192650	2.3538480
H	5.9042520	0.1792580	1.3177770
H	6.0015680	-1.8269480	-0.1585200
H	4.8072870	-2.7285860	0.8063890
H	4.5630860	-2.5032430	-0.9481220
H	5.2742680	1.9209990	-0.5895370
H	4.3339740	2.0372660	-2.0870620
H	2.2043910	2.2661700	-0.7434700
H	3.1946860	2.3170320	0.7593970
H	2.8636890	4.8592370	0.9180310

Di(α -hydroxy) Ether Dimer @ 298 K

C	-4.6941290	1.4496740	0.9948710
C	-3.4673130	0.7846820	0.4352560
C	-2.5047790	1.4988830	-0.5414360
C	-2.3948300	0.1810920	-1.3656760
C	-3.6996260	-0.3509020	-0.6437610
C	-3.7651760	-1.7762660	-0.0890590
C	-4.9264810	-0.0743000	-1.5261160
C	-1.0714500	-0.5625100	-1.1827190
O	-1.0574090	-1.8296280	-1.8699100
H	-1.8534570	-2.3187180	-1.5834080
H	-1.5709390	1.8796870	-0.1047310
H	-2.9939930	2.3066730	-1.1020200
H	-0.2741800	0.0139240	-1.6845330
H	-2.5240980	0.2998960	-2.4542330
H	-4.9297380	-0.7552400	-2.3930100
H	-5.8592960	-0.2374600	-0.9626690
H	-4.9362600	0.9577660	-1.9115100
H	-2.8753190	-2.0294340	0.5050630
H	-4.6483120	-1.8730520	0.5634940
H	-3.8896160	-2.5199940	-0.8981870
O	-4.8450180	2.7491860	0.5921760
O	-5.5118110	0.8981310	1.7228200
H	-2.9155890	0.3472530	1.2812870
O	-0.8014120	-0.7010370	0.2015310
C	0.4656390	-1.3220380	0.6204690

C	0.4196670	-1.1738720	2.1379940
O	0.4389430	-2.7158080	0.3413370
C	1.6411150	-0.6520090	-0.1188980
C	3.1506160	-0.9693380	0.2581560
C	3.1900110	0.4271190	0.9791960
C	1.9060850	0.8475130	0.2170760
C	3.9732900	-1.0113480	-1.0421010
C	3.5241120	-2.1869320	1.1085260
C	4.4572890	1.3024690	1.0002580
C	4.9185330	1.8836890	-0.3193520
O	4.2326210	2.5187730	-1.1102760
O	6.2526190	1.6663320	-0.5356510
H	6.4628230	2.1113790	-1.3849190
H	4.2573580	2.1770060	1.6458020
H	5.2902380	0.7505940	1.4623600
H	2.9326600	0.2531780	2.0386560
H	2.1243380	1.4493120	-0.6758160
H	1.1312710	1.3647140	0.8037200
H	1.4801280	-0.8488380	-1.1923370
H	-0.5433290	-1.5673210	2.4916820
H	1.2215040	-1.7513790	2.6115820
H	0.4993740	-0.1199780	2.4371750
H	3.7343520	-0.1763070	-1.7189060
H	5.0552220	-0.9849100	-0.8323280
H	3.7628470	-1.9486040	-1.5834310
H	3.2052740	-3.1226440	0.6246140
H	4.6190890	-2.2263180	1.2398310
H	3.0754480	-2.1625950	2.1112580
H	0.2352310	-2.7908520	-0.6162420
H	-5.6767330	3.0610410	1.0094360

Terpenylic Acid Dimer @ 298 K

C	-4.0552450	-0.9164180	0.8444260
C	-4.2408880	0.5799610	0.4359860
O	-4.8266370	-1.6322480	-0.1889520
C	-4.9724450	-0.8694740	-1.3234200
C	-4.3616440	0.5047100	-1.0913600
C	-4.6962590	-1.2522370	2.1884320
C	-2.6136180	-1.4309660	0.7672350
O	-5.5195510	-1.2971630	-2.3202380
C	-3.2500460	1.5973520	1.0414000
C	-1.8125020	1.5611200	0.5659290
O	-0.9236720	1.5623900	1.5469700
O	-1.5061390	1.5761430	-0.6452530
H	-5.2302060	0.8750770	0.8301590
H	-4.9966270	1.2824250	-1.5375760

H	-3.3815880	0.5533650	-1.5923410
H	-5.7616660	-0.9780290	2.1904880
H	-4.6153160	-2.3288750	2.3983540
H	-4.1903160	-0.7080320	3.0014340
H	-1.9970080	-1.0063980	1.5742880
H	-2.6147890	-2.5249190	0.8801600
H	-2.1460350	-1.1915600	-0.1995060
H	-3.6162810	2.6094560	0.7933870
H	-3.2521940	1.5222790	2.1388100
H	0.0360840	1.5782870	1.1657340
C	4.0552450	-0.9164470	-0.8443930
C	4.2408860	0.5799460	-0.4360070
O	4.8266410	-1.6322390	0.1890090
C	4.9724500	-0.8694250	1.3234490
C	4.3616460	0.5047510	1.0913410
C	4.6962570	-1.2523130	-2.1883880
C	2.6136200	-1.4309950	-0.7671810
O	5.5195590	-1.2970770	2.3202820
C	3.2500420	1.5973140	-1.0414570
C	1.8124980	1.5610990	-0.5659840
O	0.9236680	1.5623340	-1.5470250
O	1.5061360	1.5761600	0.6451980
H	5.2302040	0.8750500	-0.8301920
H	4.9966280	1.2824820	1.5375280
H	3.3815910	0.5534220	1.5923220
H	5.7616640	-0.9781020	-2.1904570
H	4.6153180	-2.3289600	-2.3982700
H	4.1903100	-0.7081400	-3.0014100
H	1.9970070	-1.0064570	-1.5742480
H	2.6147920	-2.5249520	-0.8800680
H	2.1460380	-1.1915560	0.1995520
H	3.6162750	2.6094280	-0.7934800
H	3.2521890	1.5222020	-2.1388630
H	-0.0360880	1.5782460	-1.1657890

Terpenylic Acid Dimer @ 373 K

C	-4.0552450	-0.9164180	0.8444260
C	-4.2408880	0.5799610	0.4359860
O	-4.8266370	-1.6322480	-0.1889520
C	-4.9724450	-0.8694740	-1.3234200
C	-4.3616440	0.5047100	-1.0913600
C	-4.6962590	-1.2522370	2.1884320
C	-2.6136180	-1.4309660	0.7672350
O	-5.5195510	-1.2971630	-2.3202380
C	-3.2500460	1.5973520	1.0414000
C	-1.8125020	1.5611200	0.5659290

O	-0.9236720	1.5623900	1.5469700
O	-1.5061390	1.5761430	-0.6452530
H	-5.2302060	0.8750770	0.8301590
H	-4.9966270	1.2824250	-1.5375760
H	-3.3815880	0.5533650	-1.5923410
H	-5.7616660	-0.9780290	2.1904880
H	-4.6153160	-2.3288750	2.3983540
H	-4.1903160	-0.7080320	3.0014340
H	-1.9970080	-1.0063980	1.5742880
H	-2.6147890	-2.5249190	0.8801600
H	-2.1460350	-1.1915600	-0.1995060
H	-3.6162810	2.6094560	0.7933870
H	-3.2521940	1.5222790	2.1388100
H	0.0360840	1.5782870	1.1657340
C	4.0552450	-0.9164470	-0.8443930
C	4.2408860	0.5799460	-0.4360070
O	4.8266410	-1.6322390	0.1890090
C	4.9724500	-0.8694250	1.3234490
C	4.3616460	0.5047510	1.0913410
C	4.6962570	-1.2523130	-2.1883880
C	2.6136200	-1.4309950	-0.7671810
O	5.5195590	-1.2970770	2.3202820
C	3.2500420	1.5973140	-1.0414570
C	1.8124980	1.5610990	-0.5659840
O	0.9236680	1.5623340	-1.5470250
O	1.5061360	1.5761600	0.6451980
H	5.2302040	0.8750500	-0.8301920
H	4.9966280	1.2824820	1.5375280
H	3.3815910	0.5534220	1.5923220
H	5.7616640	-0.9781020	-2.1904570
H	4.6153180	-2.3289600	-2.3982700
H	4.1903100	-0.7081400	-3.0014100
H	1.9970070	-1.0064570	-1.5742480
H	2.6147920	-2.5249520	-0.8800680
H	2.1460380	-1.1915560	0.1995520
H	3.6162750	2.6094280	-0.7934800
H	3.2521890	1.5222020	-2.1388630
H	-0.0360880	1.5782460	-1.1657890

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer alkyl carboxylate @ 298 K**

C	4.4006480	0.5665660	0.9848840
C	2.9762950	0.6442040	1.5289870
C	5.3993620	0.1473080	2.0521540
O	4.7716970	1.9621220	0.5675580
C	4.5613910	-0.2144760	-0.3523620

C	4.1735150	0.8266610	-1.4105300
C	4.6070710	2.1223110	-0.7729030
C	3.9202020	-1.6166490	-0.4257380
C	2.4155620	-1.7425050	-0.4236010
O	1.8128020	-2.4234050	0.4385680
O	1.7913230	-1.1360960	-1.4259840
O	4.8029820	3.2162840	-1.3054650
H	2.9304160	1.3933060	2.3335550
H	2.2534180	0.9261790	0.7482710
H	2.6789240	-0.3245850	1.9560910
H	5.2070060	-0.8976970	2.3401430
H	6.4305500	0.2195570	1.6752810
H	5.2996690	0.7721910	2.9523920
H	5.6438240	-0.3976110	-0.4633640
H	3.0848600	0.8812180	-1.5776820
H	4.6577310	0.6862010	-2.3861280
H	4.2644580	-2.0847230	-1.3639860
H	4.3006500	-2.2295520	0.4031340
H	0.7646300	-1.2769410	-1.3670860
C	-5.3507250	1.7386070	-0.3242720
C	-3.9378360	1.2646610	-0.1720930
C	-3.4251670	0.3527900	-1.3169420
C	-3.7368640	-0.8910380	-0.4477370
C	-3.7874990	0.0226280	0.8288260
C	-2.8908940	-2.1784210	-0.4898690
C	-1.3922710	-2.0294200	-0.4834190
C	-2.4608860	0.1425390	1.5851030
C	-4.9304660	-0.2659720	1.7994950
O	-6.1972740	1.2847580	-1.1012210
O	-5.6480750	2.7521260	0.5416740
O	-0.7700880	-2.6540670	0.5134700
O	-0.7755850	-1.4047990	-1.3790460
H	-3.3048940	2.1201580	0.1040520
H	-2.3497230	0.5061170	-1.4758430
H	-3.9499370	0.4294620	-2.2801440
H	-4.7708050	-1.2116880	-0.6568810
H	-3.1872780	-2.8398500	0.3374330
H	-3.1270810	-2.7051140	-1.4311820
H	-1.6147790	0.3634240	0.9153960
H	-2.5220990	0.9575480	2.3245630
H	-2.2387000	-0.7887590	2.1303470
H	-4.7634580	-1.2387630	2.2916080
H	-4.9914140	0.5003850	2.5895090
H	-5.9048690	-0.3154210	1.2872670
H	-6.5962640	2.9824790	0.4187030
H	0.2542950	-2.5416710	0.4382230

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer alkyl carboxylate @ 373 K**

C	4.4006480	0.5665660	0.9848840
C	2.9762950	0.6442040	1.5289870
C	5.3993620	0.1473080	2.0521540
O	4.7716970	1.9621220	0.5675580
C	4.5613910	-0.2144760	-0.3523620
C	4.1735150	0.8266610	-1.4105300
C	4.6070710	2.1223110	-0.7729030
C	3.9202020	-1.6166490	-0.4257380
C	2.4155620	-1.7425050	-0.4236010
O	1.8128020	-2.4234050	0.4385680
O	1.7913230	-1.1360960	-1.4259840
O	4.8029820	3.2162840	-1.3054650
H	2.9304160	1.3933060	2.3335550
H	2.2534180	0.9261790	0.7482710
H	2.6789240	-0.3245850	1.9560910
H	5.2070060	-0.8976970	2.3401430
H	6.4305500	0.2195570	1.6752810
H	5.2996690	0.7721910	2.9523920
H	5.6438240	-0.3976110	-0.4633640
H	3.0848600	0.8812180	-1.5776820
H	4.6577310	0.6862010	-2.3861280
H	4.2644580	-2.0847230	-1.3639860
H	4.3006500	-2.2295520	0.4031340
H	0.7646300	-1.2769410	-1.3670860
C	-5.3507250	1.7386070	-0.3242720
C	-3.9378360	1.2646610	-0.1720930
C	-3.4251670	0.3527900	-1.3169420
C	-3.7368640	-0.8910380	-0.4477370
C	-3.7874990	0.0226280	0.8288260
C	-2.8908940	-2.1784210	-0.4898690
C	-1.3922710	-2.0294200	-0.4834190
C	-2.4608860	0.1425390	1.5851030
C	-4.9304660	-0.2659720	1.7994950
O	-6.1972740	1.2847580	-1.1012210
O	-5.6480750	2.7521260	0.5416740
O	-0.7700880	-2.6540670	0.5134700
O	-0.7755850	-1.4047990	-1.3790460
H	-3.3048940	2.1201580	0.1040520
H	-2.3497230	0.5061170	-1.4758430
H	-3.9499370	0.4294620	-2.2801440
H	-4.7708050	-1.2116880	-0.6568810
H	-3.1872780	-2.8398500	0.3374330
H	-3.1270810	-2.7051140	-1.4311820
H	-1.6147790	0.3634240	0.9153960

H	-2.5220990	0.9575480	2.3245630
H	-2.2387000	-0.7887590	2.1303470
H	-4.7634580	-1.2387630	2.2916080
H	-4.9914140	0.5003850	2.5895090
H	-5.9048690	-0.3154210	1.2872670
H	-6.5962640	2.9824790	0.4187030
H	0.2542950	-2.5416710	0.4382230

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer carboxylate @ 298 K**

C	-1.4172320	-1.3600970	-0.4762180
C	-2.8978270	-1.2911140	-0.2735480
C	-3.6840200	-0.4689180	-1.3280820
C	-3.6980210	0.7408760	-0.3609200
C	-3.3397420	-0.2157520	0.8322490
C	-4.8736000	1.7309020	-0.2773010
C	-6.2675050	1.1574700	-0.2352150
C	-4.5463680	-0.7554410	1.6059620
C	-2.2791090	0.3063020	1.7999140
O	-0.7802480	-0.5782190	-1.2218770
O	-0.8189860	-2.3146790	0.2389830
O	-7.0007320	1.6274200	0.8142240
O	-6.7532400	0.3883580	-1.0695280
H	-3.2665560	-2.3040670	-0.0587950
H	-4.6805940	-0.9016320	-1.4856000
H	-3.1943290	-0.3193660	-2.3010490
H	-2.8069680	1.3581030	-0.5620290
H	-4.7299610	2.4018560	0.5822880
H	-4.8517710	2.3604570	-1.1848320
H	-5.3211140	-1.1690320	0.9417840
H	-4.2267340	-1.5605840	2.2873980
H	-5.0019620	0.0397630	2.2180360
H	-2.6919370	1.1471440	2.3819680
H	-1.9684490	-0.4733090	2.5147560
H	-1.3832500	0.6738890	1.2743250
H	0.2028840	-2.2861750	0.1074170
H	-7.9043690	1.2447390	0.7444640
C	4.8026930	0.1780490	0.9308810
C	3.4519410	0.2983590	1.6325040
C	5.8180250	-0.5817650	1.7702290
O	5.3272660	1.5776740	0.7778880
C	4.7446440	-0.3020710	-0.5494500
C	4.4314910	0.9864180	-1.3221550
C	5.0833260	2.0489650	-0.4741350
C	3.9031680	-1.5623890	-0.8384970
C	2.4000850	-1.5071990	-0.7020620
O	1.7727200	-2.3289300	0.0055090

O	1.7948690	-0.5781950	-1.4320910
O	5.3844650	3.2038100	-0.7815230
H	3.5792860	0.8307450	2.5869510
H	2.7200270	0.8493490	1.0224140
H	3.0479920	-0.6998610	1.8566470
H	5.5041540	-1.6332620	1.8582520
H	6.8132210	-0.5543340	1.3020120
H	5.8858780	-0.1604150	2.7845170
H	5.7769550	-0.5913860	-0.8108610
H	3.3521450	1.2069270	-1.3668570
H	4.8226290	1.0081700	-2.3481240
H	4.0979110	-1.8533390	-1.8856260
H	4.2581620	-2.3861430	-0.2037840
H	0.7661590	-0.6217190	-1.3132930

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer carboxylate @ 373 K**

C	-1.4172320	-1.3600970	-0.4762180
C	-2.8978270	-1.2911140	-0.2735480
C	-3.6840200	-0.4689180	-1.3280820
C	-3.6980210	0.7408760	-0.3609200
C	-3.3397420	-0.2157520	0.8322490
C	-4.8736000	1.7309020	-0.2773010
C	-6.2675050	1.1574700	-0.2352150
C	-4.5463680	-0.7554410	1.6059620
C	-2.2791090	0.3063020	1.7999140
O	-0.7802480	-0.5782190	-1.2218770
O	-0.8189860	-2.3146790	0.2389830
O	-7.0007320	1.6274200	0.8142240
O	-6.7532400	0.3883580	-1.0695280
H	-3.2665560	-2.3040670	-0.0587950
H	-4.6805940	-0.9016320	-1.4856000
H	-3.1943290	-0.3193660	-2.3010490
H	-2.8069680	1.3581030	-0.5620290
H	-4.7299610	2.4018560	0.5822880
H	-4.8517710	2.3604570	-1.1848320
H	-5.3211140	-1.1690320	0.9417840
H	-4.2267340	-1.5605840	2.2873980
H	-5.0019620	0.0397630	2.2180360
H	-2.6919370	1.1471440	2.3819680
H	-1.9684490	-0.4733090	2.5147560
H	-1.3832500	0.6738890	1.2743250
H	0.2028840	-2.2861750	0.1074170
H	-7.9043690	1.2447390	0.7444640
C	4.8026930	0.1780490	0.9308810
C	3.4519410	0.2983590	1.6325040
C	5.8180250	-0.5817650	1.7702290

O	5.3272660	1.5776740	0.7778880
C	4.7446440	-0.3020710	-0.5494500
C	4.4314910	0.9864180	-1.3221550
C	5.0833260	2.0489650	-0.4741350
C	3.9031680	-1.5623890	-0.8384970
C	2.4000850	-1.5071990	-0.7020620
O	1.7727200	-2.3289300	0.0055090
O	1.7948690	-0.5781950	-1.4320910
O	5.3844650	3.2038100	-0.7815230
H	3.5792860	0.8307450	2.5869510
H	2.7200270	0.8493490	1.0224140
H	3.0479920	-0.6998610	1.8566470
H	5.5041540	-1.6332620	1.8582520
H	6.8132210	-0.5543340	1.3020120
H	5.8858780	-0.1604150	2.7845170
H	5.7769550	-0.5913860	-0.8108610
H	3.3521450	1.2069270	-1.3668570
H	4.8226290	1.0081700	-2.3481240
H	4.0979110	-1.8533390	-1.8856260
H	4.2581620	-2.3861430	-0.2037840
H	0.7661590	-0.6217190	-1.3132930

Cartesian coordinates for optimized monomers and dimers in the methanol solvent continuum studied in the article

***cis*-Pinic Acid @ 298 K**

C	-2.6403890	-0.4775140	-0.1418020
C	-1.2726520	-0.3026110	-0.7303150
C	-0.2358060	-1.3788000	-0.3155020
C	0.3210730	-0.4117650	0.7591570
C	-0.3842710	0.7912700	0.0334470
C	1.8109540	-0.3716820	1.1499680
C	2.8188510	-0.3653260	0.0277090
C	0.4880520	1.5320350	-0.9853190
C	-1.0949120	1.7860320	0.9496250
O	-2.9395640	-1.2033240	0.8109890
O	-3.5658940	0.3009060	-0.7643200
O	3.6643170	0.6959290	0.0802250
O	2.9261010	-1.2379250	-0.8379010
H	-1.3753640	-0.0997530	-1.8063840
H	0.4729060	-1.5665130	-1.1333020
H	-0.6380040	-2.3378350	0.0427200
H	-0.2248060	-0.5865830	1.7013890
H	1.9974760	0.4849070	1.8146000
H	2.0305070	-1.2867650	1.7288920
H	1.0061170	0.8456470	-1.6739220
H	-0.1358230	2.2046880	-1.5970950
H	1.2459140	2.1504260	-0.4773440
H	-0.3502860	2.3598640	1.5271670
H	-1.6966910	2.5087700	0.3736680
H	-1.7572420	1.2833520	1.6732700
H	-4.4291220	0.1754000	-0.3091680
H	4.3093400	0.6098750	-0.6582420

***cis*-Pinic Acid @ 373 K**

C	-2.6403890	-0.4775140	-0.1418020
C	-1.2726520	-0.3026110	-0.7303150
C	-0.2358060	-1.3788000	-0.3155020
C	0.3210730	-0.4117650	0.7591570
C	-0.3842710	0.7912700	0.0334470
C	1.8109540	-0.3716820	1.1499680
C	2.8188510	-0.3653260	0.0277090
C	0.4880520	1.5320350	-0.9853190
C	-1.0949120	1.7860320	0.9496250
O	-2.9395640	-1.2033240	0.8109890
O	-3.5658940	0.3009060	-0.7643200

O	3.6643170	0.6959290	0.0802250
O	2.9261010	-1.2379250	-0.8379010
H	-1.3753640	-0.0997530	-1.8063840
H	0.4729060	-1.5665130	-1.1333020
H	-0.6380040	-2.3378350	0.0427200
H	-0.2248060	-0.5865830	1.7013890
H	1.9974760	0.4849070	1.8146000
H	2.0305070	-1.2867650	1.7288920
H	1.0061170	0.8456470	-1.6739220
H	-0.1358230	2.2046880	-1.5970950
H	1.2459140	2.1504260	-0.4773440
H	-0.3502860	2.3598640	1.5271670
H	-1.6966910	2.5087700	0.3736680
H	-1.7572420	1.2833520	1.6732700
H	-4.4291220	0.1754000	-0.3091680
H	4.3093400	0.6098750	-0.6582420

Pinonaldehyde @ 298 K

C	-2.3563930	0.3999340	-0.6814050
C	-2.6491440	-0.9329830	-0.0592000
O	2.9231490	-0.5839400	-1.0717410
C	2.1792020	-0.7201690	-0.0851600
C	2.7384420	-1.0628320	1.2719190
C	0.6885990	-0.5387140	-0.1831320
C	0.0165080	-0.3387420	-1.5570630
C	-0.8860980	0.7760270	-0.9509030
C	0.0951960	0.8717140	0.2825640
C	-0.4928890	0.9189790	1.6894140
C	1.0838620	2.0270540	0.0789770
O	-3.5373030	-1.1220510	0.7797580
H	-2.8790400	1.1844920	-0.1107150
H	-2.8537780	0.3396240	-1.6729910
H	-2.0613250	-1.8053220	-0.4271530
H	3.8225240	-0.8887120	1.3071470
H	2.2294840	-0.4963620	2.0678520
H	2.5416130	-2.1314690	1.4715460
H	0.2011150	-1.3287190	0.4137930
H	-0.4865510	-1.2167790	-1.9899950
H	0.7211430	0.0608280	-2.3013470
H	-0.9053750	1.7082870	-1.5386870
H	-1.1826060	0.0849210	1.8908340
H	0.3095830	0.8731440	2.4450050
H	-1.0426310	1.8620190	1.8507080
H	0.5602960	2.9901820	0.2003940
H	1.9004870	1.9934310	0.8197380

H	1.5345810	2.0167470	-0.9263330
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Pinonaldehyde @ 373 K

C	-2.3563930	0.3999340	-0.6814050
C	-2.6491440	-0.9329830	-0.0592000
O	2.9231490	-0.5839400	-1.0717410
C	2.1792020	-0.7201690	-0.0851600
C	2.7384420	-1.0628320	1.2719190
C	0.6885990	-0.5387140	-0.1831320
C	0.0165080	-0.3387420	-1.5570630
C	-0.8860980	0.7760270	-0.9509030
C	0.0951960	0.8717140	0.2825640
C	-0.4928890	0.9189790	1.6894140
C	1.0838620	2.0270540	0.0789770
O	-3.5373030	-1.1220510	0.7797580
H	-2.8790400	1.1844920	-0.1107150
H	-2.8537780	0.3396240	-1.6729910
H	-2.0613250	-1.8053220	-0.4271530
H	3.8225240	-0.8887120	1.3071470
H	2.2294840	-0.4963620	2.0678520
H	2.5416130	-2.1314690	1.4715460
H	0.2011150	-1.3287190	0.4137930
H	-0.4865510	-1.2167790	-1.9899950
H	0.7211430	0.0608280	-2.3013470
H	-0.9053750	1.7082870	-1.5386870
H	-1.1826060	0.0849210	1.8908340
H	0.3095830	0.8731440	2.4450050
H	-1.0426310	1.8620190	1.8507080
H	0.5602960	2.9901820	0.2003940
H	1.9004870	1.9934310	0.8197380
H	1.5345810	2.0167470	-0.9263330

***cis*-Pinonic Acid @ 298 K**

C	-2.8699520	-0.1817590	-0.3905300
C	-1.8740770	-0.8979620	0.4866060
C	-0.4163060	-0.7373970	0.0632920
C	0.6495070	-1.4552580	0.9271570
C	1.5943610	-0.2357410	0.7899510
C	0.3355880	0.6284960	0.2833270
C	0.5120900	1.5002720	-0.9604870
C	-0.2172840	1.4640270	1.4417560
O	-2.7123610	0.1016540	-1.5795360
O	-4.0218390	0.1049110	0.2696480
H	-4.6441470	0.5273780	-0.3646440

H	-2.0361860	-0.5969220	1.5331870
H	-2.1457530	-1.9702850	0.4360990
H	-0.3068390	-1.0352530	-0.9923020
H	1.0316590	-2.4121360	0.5412790
H	0.3231230	-1.5912010	1.9696100
H	2.0247190	0.1633070	1.7223580
H	-0.3412600	0.8737960	2.3636420
H	0.4652860	2.3002070	1.6671660
H	-1.1988030	1.8936500	1.1769950
H	-0.4626920	1.9155090	-1.2659310
H	1.1873500	2.3502020	-0.7654370
H	0.9103950	0.9299880	-1.8151090
C	2.6922180	-0.3595290	-0.2342830
O	2.6884030	-1.2462180	-1.1063850
C	3.8068900	0.6523770	-0.1613540
H	4.4049090	0.6507570	-1.0827340
H	3.4164620	1.6619340	0.0425930
H	4.4599410	0.3911440	0.6908070

***cis*-Pinonic Acid @ 373 K**

C	-2.8699520	-0.1817590	-0.3905300
C	-1.8740770	-0.8979620	0.4866060
C	-0.4163060	-0.7373970	0.0632920
C	0.6495070	-1.4552580	0.9271570
C	1.5943610	-0.2357410	0.7899510
C	0.3355880	0.6284960	0.2833270
C	0.5120900	1.5002720	-0.9604870
C	-0.2172840	1.4640270	1.4417560
O	-2.7123610	0.1016540	-1.5795360
O	-4.0218390	0.1049110	0.2696480
H	-4.6441470	0.5273780	-0.3646440
H	-2.0361860	-0.5969220	1.5331870
H	-2.1457530	-1.9702850	0.4360990
H	-0.3068390	-1.0352530	-0.9923020
H	1.0316590	-2.4121360	0.5412790
H	0.3231230	-1.5912010	1.9696100
H	2.0247190	0.1633070	1.7223580
H	-0.3412600	0.8737960	2.3636420
H	0.4652860	2.3002070	1.6671660
H	-1.1988030	1.8936500	1.1769950
H	-0.4626920	1.9155090	-1.2659310
H	1.1873500	2.3502020	-0.7654370
H	0.9103950	0.9299880	-1.8151090
C	2.6922180	-0.3595290	-0.2342830
O	2.6884030	-1.2462180	-1.1063850

C	3.8068900	0.6523770	-0.1613540
H	4.4049090	0.6507570	-1.0827340
H	3.4164620	1.6619340	0.0425930
H	4.4599410	0.3911440	0.6908070

Hydroperoxide Monomer @ 298 K

C	-2.2530580	-1.1023130	-0.3402330
C	-0.9182060	-0.4152100	-0.1908830
C	-0.0403760	-0.5995710	1.0750680
C	0.3441050	0.9113900	1.0092090
C	-0.8365410	1.1513280	-0.0217610
C	-0.5461050	1.9534510	-1.2898850
C	-2.0530810	1.7407530	0.7069880
C	1.7784650	1.2768180	0.5867390
C	2.4987070	0.3956440	-0.4415530
O	3.1212110	-0.6740360	0.3106750
O	3.8556100	-1.5249610	-0.6392920
C	-2.4941180	-2.3732270	0.4299940
O	-3.1213520	-0.6360260	-1.0997190
H	-0.3491960	-0.7102010	-1.0933110
H	0.7833200	-1.3237310	0.9964560
H	-0.6314020	-0.8379460	1.9720210
H	0.1494460	1.4448690	1.9549700
H	0.3236480	1.5673820	-1.8441320
H	-1.4142770	1.9172040	-1.9696600
H	-0.3544150	3.0143560	-1.0537490
H	-1.8291880	2.7715630	1.0304870
H	-2.9420810	1.7775270	0.0569650
H	-2.3163820	1.1586410	1.6061950
H	1.7834930	2.3079340	0.1936830
H	2.4185470	1.3093470	1.4870210
H	1.8219800	-0.0404210	-1.1955040
H	3.2889570	0.9664010	-0.9589920
H	3.1888990	-2.2216030	-0.8327380
H	-3.3865870	-2.8921090	0.0547230
H	-1.6147650	-3.0363060	0.3837210
H	-2.6425110	-2.1270950	1.4964390

Hydroperoxide Monomer @ 373 K

C	-2.2530580	-1.1023130	-0.3402330
C	-0.9182060	-0.4152100	-0.1908830
C	-0.0403760	-0.5995710	1.0750680
C	0.3441050	0.9113900	1.0092090
C	-0.8365410	1.1513280	-0.0217610

C	-0.5461050	1.9534510	-1.2898850
C	-2.0530810	1.7407530	0.7069880
C	1.7784650	1.2768180	0.5867390
C	2.4987070	0.3956440	-0.4415530
O	3.1212110	-0.6740360	0.3106750
O	3.8556100	-1.5249610	-0.6392920
C	-2.4941180	-2.3732270	0.4299940
O	-3.1213520	-0.6360260	-1.0997190
H	-0.3491960	-0.7102010	-1.0933110
H	0.7833200	-1.3237310	0.9964560
H	-0.6314020	-0.8379460	1.9720210
H	0.1494460	1.4448690	1.9549700
H	0.3236480	1.5673820	-1.8441320
H	-1.4142770	1.9172040	-1.9696600
H	-0.3544150	3.0143560	-1.0537490
H	-1.8291880	2.7715630	1.0304870
H	-2.9420810	1.7775270	0.0569650
H	-2.3163820	1.1586410	1.6061950
H	1.7834930	2.3079340	0.1936830
H	2.4185470	1.3093470	1.4870210
H	1.8219800	-0.0404210	-1.1955040
H	3.2889570	0.9664010	-0.9589920
H	3.1888990	-2.2216030	-0.8327380
H	-3.3865870	-2.8921090	0.0547230
H	-1.6147650	-3.0363060	0.3837210
H	-2.6425110	-2.1270950	1.4964390

Terpenylic Acid @ 298 K

C	0.7009190	1.0202150	-0.0854220
C	-0.0190020	1.0978660	-1.4305480
C	0.9473210	2.3975810	0.5116730
O	2.0516140	0.4253950	-0.3625570
C	0.1088770	0.0006540	0.9336990
C	0.7427570	-1.3302670	0.5056670
C	2.0688420	-0.8984160	-0.0690180
C	-1.4158060	0.0510160	1.1681110
C	-2.3593730	-0.3273570	0.0492180
O	-3.2616900	0.3963360	-0.3773920
O	-2.1727120	-1.5865610	-0.4130490
O	3.0722340	-1.5784770	-0.2838880
H	0.6014670	1.6584150	-2.1464580
H	-0.2157210	0.1000370	-1.8525040
H	-0.9740380	1.6336310	-1.3247890
H	-0.0139380	2.8531720	0.7965250
H	1.5772640	2.3294040	1.4116380

H	1.4358440	3.0618330	-0.2175930
H	0.5484640	0.2633960	1.9116010
H	0.1787770	-1.8392150	-0.2939690
H	0.8848580	-2.0489220	1.3245880
H	-1.6428430	-0.6338610	2.0040390
H	-1.6987530	1.0622030	1.4927660
H	-2.8441600	-1.7613900	-1.1110320

Terpenylic Acid @ 373 K

C	0.7009190	1.0202150	-0.0854220
C	-0.0190020	1.0978660	-1.4305480
C	0.9473210	2.3975810	0.5116730
O	2.0516140	0.4253950	-0.3625570
C	0.1088770	0.0006540	0.9336990
C	0.7427570	-1.3302670	0.5056670
C	2.0688420	-0.8984160	-0.0690180
C	-1.4158060	0.0510160	1.1681110
C	-2.3593730	-0.3273570	0.0492180
O	-3.2616900	0.3963360	-0.3773920
O	-2.1727120	-1.5865610	-0.4130490
O	3.0722340	-1.5784770	-0.2838880
H	0.6014670	1.6584150	-2.1464580
H	-0.2157210	0.1000370	-1.8525040
H	-0.9740380	1.6336310	-1.3247890
H	-0.0139380	2.8531720	0.7965250
H	1.5772640	2.3294040	1.4116380
H	1.4358440	3.0618330	-0.2175930
H	0.5484640	0.2633960	1.9116010
H	0.1787770	-1.8392150	-0.2939690
H	0.8848580	-2.0489220	1.3245880
H	-1.6428430	-0.6338610	2.0040390
H	-1.6987530	1.0622030	1.4927660
H	-2.8441600	-1.7613900	-1.1110320

***cis*-Pinic Acid Dimer @ 298 K**

O	6.2966380	-1.8009820	-0.2704620
C	6.9440820	-0.7686760	-0.1111240
C	6.5475590	0.4221620	0.7372130
C	5.0650930	0.6838780	1.0339110
C	4.1633560	-0.4975160	1.5034990
C	3.4142840	-0.4646150	0.1546970
C	4.0713470	0.9521360	-0.1655610
C	3.1453480	2.1302860	0.1635050
C	4.6354510	1.1028140	-1.5763520

C	1.9198770	-0.5343640	0.1300240
O	8.1735620	-0.6982670	-0.6977750
O	1.2058720	-0.5235430	1.1585150
O	1.4064870	-0.5764340	-1.0989500
H	6.9994350	1.3304240	0.3036980
H	7.0725080	0.2640850	1.6995070
H	5.0629000	1.5268790	1.7439980
H	3.5187310	-0.2102690	2.3469740
H	4.6653480	-1.4442850	1.7445430
H	3.8052880	-1.2079780	-0.5562930
H	2.7128670	2.0464920	1.1738180
H	3.7132580	3.0747890	0.1212410
H	2.3156350	2.2045960	-0.5596580
H	3.8134660	1.1362030	-2.3112970
H	5.2052140	2.0424750	-1.6737230
H	5.2941480	0.2686710	-1.8625700
H	8.5990190	0.1688530	-0.5279570
H	0.3776700	-0.5637900	-1.0693540
O	-6.2966380	-1.8009900	0.2704470
C	-6.9440790	-0.7686790	0.1111240
C	-6.5475610	0.4221570	-0.7372180
C	-5.0650940	0.6838750	-1.0339150
C	-4.1633560	-0.4975180	-1.5034990
C	-3.4142850	-0.4646130	-0.1546960
C	-4.0713510	0.9521380	0.1655580
C	-3.1453530	2.1302890	-0.1635090
C	-4.6354560	1.1028170	1.5763480
C	-1.9198780	-0.5343580	-0.1300220
O	-8.1735460	-0.6982640	0.6977980
O	-1.2058720	-0.5235380	-1.1585130
O	-1.4064880	-0.5764300	1.0989520
H	-6.9994380	1.3304220	-0.3037070
H	-7.0725060	0.2640760	-1.6995120
H	-5.0629020	1.5268750	-1.7440040
H	-3.5187310	-0.2102730	-2.3469740
H	-4.6653470	-1.4442890	-1.7445400
H	-3.8052890	-1.2079740	0.5562950
H	-2.7128720	2.0464950	-1.1738220
H	-3.7132630	3.0747910	-0.1212440
H	-2.3156390	2.2045990	0.5596540
H	-3.8134720	1.1362090	2.3112940
H	-5.2052220	2.0424770	1.6737180
H	-5.2941520	0.2686730	1.8625670
H	-8.5990040	0.1688560	0.5279870
H	-0.3776720	-0.5637860	1.0693570

***cis*-Pinic Acid Dimer @ 373 K**

Symbol	X	Y	Z
O	6.2966290	-1.8009880	-0.2704530
C	6.9440800	-0.7686850	-0.1111190
C	6.5475620	0.4221610	0.7372070
C	5.0650980	0.6838880	1.0339030
C	4.1633570	-0.4974980	1.5035040
C	3.4142860	-0.4646100	0.1547020
C	4.0713520	0.9521370	-0.1655710
C	3.1453560	2.1302920	0.1634850
C	4.6354550	1.1028000	-1.5763630
C	1.9198790	-0.5343560	0.1300290
O	8.1735630	-0.6982880	-0.6977660
O	1.2058740	-0.5235260	1.1585200
O	1.4064880	-0.5764370	-1.0989450
H	6.9994430	1.3304190	0.3036850
H	7.0725100	0.2640920	1.6995020
H	5.0629090	1.5268960	1.7439810
H	3.5187330	-0.2102400	2.3469760
H	4.6653470	-1.4442660	1.7445590
H	3.8052890	-1.2079810	-0.5562810
H	2.7128750	2.0465090	1.1737990
H	3.7132670	3.0747930	0.1212120
H	2.3156420	2.2045970	-0.5596790
H	3.8134710	1.1361850	-2.3113080
H	5.2052220	2.0424590	-1.6737430
H	5.2941500	0.2686530	-1.8625740
H	8.5990250	0.1688290	-0.5279510
H	0.3776710	-0.5637910	-1.0693490
O	-6.2966400	-1.8009930	0.2704530
C	-6.9440820	-0.7686830	0.1111230
C	-6.5475620	0.4221500	-0.7372200
C	-5.0650950	0.6838710	-1.0339150
C	-4.1633540	-0.4975220	-1.5034950
C	-3.4142840	-0.4646120	-0.1546920
C	-4.0713530	0.9521380	0.1655590
C	-3.1453570	2.1302890	-0.1635100
C	-4.6354610	1.1028200	1.5763470
C	-1.9198770	-0.5343540	-0.1300170
O	-8.1735540	-0.6982680	0.6977870
O	-1.2058710	-0.5235380	-1.1585070
O	-1.4064880	-0.5764190	1.0989580
H	-6.9994420	1.3304160	-0.3037150
H	-7.0725030	0.2640660	-1.6995160
H	-5.0629040	1.5268690	-1.7440060

H	-3.5187290	-0.2102780	-2.3469700
H	-4.6653430	-1.4442940	-1.7445340
H	-3.8052870	-1.2079730	0.5563020
H	-2.7128750	2.0464940	-1.1738230
H	-3.7132690	3.0747910	-0.1212480
H	-2.3156440	2.2046030	0.5596530
H	-3.8134780	1.1362160	2.3112950
H	-5.2052290	2.0424790	1.6737140
H	-5.2941550	0.2686760	1.8625680
H	-8.5990130	0.1688490	0.5279660
H	-0.3776710	-0.5637730	1.0693620

Aldol Addition Dimer @ 298 K

C	-5.0858570	1.5949880	0.0980380
C	-4.7773300	2.5360810	-1.0360260
O	-6.2303970	1.5483630	0.5863560
C	-4.0140820	0.6918620	0.6610870
C	-2.5294540	0.9501170	0.2806740
C	-2.5860170	-0.2357620	-0.7165240
C	-3.9219570	-0.7421880	-0.0566010
C	-3.7166830	-1.8252980	1.0093880
C	-5.0454810	-1.1352070	-1.0143590
C	-1.4204770	-1.1736670	-0.9278460
O	-1.6223890	-2.3551460	-1.2537600
C	-0.0067820	-0.6167460	-0.8408500
C	0.8618710	-1.1582340	0.3294740
O	0.1197530	-0.8441350	1.5408020
C	2.2479100	-0.4740350	0.2850250
C	3.2648270	-0.7197410	1.4316130
C	3.8130560	0.7236300	1.2308250
C	2.5181590	1.0804120	0.3925510
C	2.7091010	1.8093570	-0.9409770
C	1.5537720	1.8848750	1.2773650
C	5.2032510	0.9075310	0.5950380
C	5.5418170	0.1651630	-0.6759430
O	6.2267280	0.9472430	-1.5539030
O	5.3088240	-1.0208970	-0.9169840
H	-4.1607600	3.3682350	-0.6520900
H	-4.1859120	2.0470550	-1.8258330
H	-5.7054650	2.9463350	-1.4556360
H	-4.2154150	0.5923540	1.7389760
H	-1.8660170	0.7515370	1.1330950
H	-2.2849780	1.9365670	-0.1374320
H	-2.8112860	0.1469260	-1.7319740
H	-2.8898530	-1.5777440	1.6943460

H	-4.6351260	-1.9359000	1.6090160
H	-3.4927420	-2.7987580	0.5455880
H	-4.7949540	-2.0859370	-1.5135640
H	-5.9957620	-1.2794640	-0.4736890
H	-5.2092040	-0.3798650	-1.7998270
H	0.5039020	-0.8866700	-1.7800030
H	-0.0440560	0.4803700	-0.7770460
H	0.6195060	-1.2076970	2.2977220
H	2.7107810	-0.8104830	-0.6584680
H	3.9708590	-1.5517100	1.2969980
H	2.7867350	-0.8234750	2.4196310
H	3.8575650	1.3004460	2.1696510
H	3.3581400	1.2546840	-1.6374000
H	1.7385370	1.9498880	-1.4466600
H	3.1484280	2.8105420	-0.7899280
H	1.9710520	2.8942200	1.4411960
H	0.5641250	2.0059880	0.8086920
H	1.4041200	1.4207840	2.2640410
H	5.4002510	1.9781930	0.4348860
H	5.9570210	0.5600780	1.3273440
H	6.4741010	0.3923500	-2.3282420
C	1.0642170	-2.6806270	0.2603610
H	0.1037180	-3.2110330	0.3265630
H	1.5626440	-2.9773740	-0.6758980
H	1.6967210	-3.0089400	1.1019770

Aldol Addition Dimer @ 373 K

C	-5.0858570	1.5949890	0.0980370
C	-4.7773300	2.5360810	-1.0360260
O	-6.2303970	1.5483630	0.5863560
C	-4.0140820	0.6918620	0.6610870
C	-2.5294540	0.9501170	0.2806740
C	-2.5860170	-0.2357620	-0.7165240
C	-3.9219570	-0.7421880	-0.0566000
C	-3.7166830	-1.8252980	1.0093880
C	-5.0454810	-1.1352070	-1.0143590
C	-1.4204770	-1.1736670	-0.9278460
O	-1.6223890	-2.3551460	-1.2537600
C	-0.0067820	-0.6167460	-0.8408500
C	0.8618710	-1.1582340	0.3294740
O	0.1197530	-0.8441350	1.5408020
C	2.2479100	-0.4740350	0.2850250
C	3.2648270	-0.7197410	1.4316130
C	3.8130560	0.7236300	1.2308250
C	2.5181590	1.0804120	0.3925510

C	2.7091010	1.8093570	-0.9409770
C	1.5537720	1.8848750	1.2773660
C	5.2032510	0.9075310	0.5950380
C	5.5418170	0.1651630	-0.6759430
O	6.2267280	0.9472430	-1.5539030
O	5.3088240	-1.0208970	-0.9169840
H	-4.1607600	3.3682350	-0.6520900
H	-4.1859120	2.0470550	-1.8258330
H	-5.7054650	2.9463350	-1.4556360
H	-4.2154150	0.5923540	1.7389760
H	-1.8660170	0.7515370	1.1330950
H	-2.2849780	1.9365670	-0.1374320
H	-2.8112860	0.1469260	-1.7319730
H	-2.8898530	-1.5777440	1.6943460
H	-4.6351260	-1.9359000	1.6090160
H	-3.4927420	-2.7987580	0.5455880
H	-4.7949540	-2.0859370	-1.5135640
H	-5.9957620	-1.2794640	-0.4736890
H	-5.2092040	-0.3798650	-1.7998270
H	0.5039020	-0.8866700	-1.7800030
H	-0.0440560	0.4803700	-0.7770460
H	0.6195060	-1.2076980	2.2977220
H	2.7107810	-0.8104830	-0.6584680
H	3.9708590	-1.5517100	1.2969980
H	2.7867350	-0.8234750	2.4196310
H	3.8575650	1.3004460	2.1696510
H	3.3581400	1.2546840	-1.6374000
H	1.7385370	1.9498880	-1.4466600
H	3.1484280	2.8105420	-0.7899280
H	1.9710520	2.8942190	1.4411960
H	0.5641250	2.0059880	0.8086920
H	1.4041200	1.4207840	2.2640420
H	5.4002510	1.9781930	0.4348860
H	5.9570210	0.5600780	1.3273440
H	6.4741010	0.3923500	-2.3282420
C	1.0642170	-2.6806270	0.2603610
H	0.1037180	-3.2110330	0.3265630
H	1.5626450	-2.9773740	-0.6758980
H	1.6967210	-3.0089400	1.1019760

Peroxyhemiacetal Dimer @ 298 K

C	-4.2066860	2.7807910	1.4007880
C	-4.7181900	1.3755570	1.2317020
O	-5.8218450	1.0319010	1.6935190
C	-3.8551290	0.3740610	0.5033220

C	-2.7139500	0.8102910	-0.4514670
C	-3.1028940	-0.3479510	-1.4223870
C	-4.4762840	-0.5124780	-0.6487050
C	-4.9306050	-1.9175880	-0.2554640
C	-5.5973570	0.2079370	-1.4116130
C	-2.1600650	-1.5611600	-1.5152540
C	-1.4143830	-2.0262160	-0.2564470
O	-0.2097910	-1.2336880	-0.1839930
O	0.4807080	-1.6269240	1.0768520
C	1.8920330	-1.9736010	0.7655340
O	2.3643180	-2.2856260	2.0642460
C	1.9208020	-3.2479470	-0.0600620
C	2.6002240	-0.7309500	0.2006360
C	2.5911890	-0.3765320	-1.3087870
C	3.9973370	0.2727400	-1.1365670
C	4.1721020	-0.5597430	0.1981980
C	4.7843050	0.1262570	1.4219930
C	4.9695790	-1.8370670	-0.1101130
C	4.0572920	1.8138750	-1.0874280
C	2.9308570	2.5394430	-0.3473290
O	3.1770180	3.9440730	-0.5901700
O	2.0985000	4.7100180	0.0545130
H	-3.1519400	2.7766390	1.7216690
H	-4.2329640	3.2974690	0.4251170
H	-4.8239340	3.3377610	2.1184970
H	-3.4604390	-0.2930760	1.2927150
H	-1.6960710	0.7868260	-0.0371900
H	-2.8878310	1.8001190	-0.8992920
H	-3.2754330	-0.0046520	-2.4566850
H	-4.1588620	-2.4716970	0.3010350
H	-5.8270530	-1.8633540	0.3849640
H	-5.1975950	-2.5104820	-1.1473400
H	-5.8219970	-0.3334660	-2.3462580
H	-6.5265650	0.2568720	-0.8207370
H	-5.3146470	1.2387800	-1.6839360
H	-2.7306930	-2.4266550	-1.8939180
H	-1.3963220	-1.3591980	-2.2879370
H	-1.9986390	-1.8832320	0.6678760
H	-1.1414310	-3.0928440	-0.3387510
H	2.5062080	-1.4496850	2.5544900
H	2.9522670	-3.5576220	-0.2729520
H	1.4190840	-4.0520630	0.4985980
H	1.3991910	-3.0983160	-1.0153390
H	2.1869630	0.1179640	0.7741130
H	1.7708470	0.2588960	-1.6736410
H	2.6416280	-1.2741230	-1.9434640

H	4.7284650	-0.0327380	-1.9042500
H	4.2290850	1.0261720	1.7271130
H	4.7988690	-0.5622740	2.2843440
H	5.8290210	0.4218200	1.2244760
H	6.0301400	-1.5744880	-0.2659560
H	4.9234750	-2.5599670	0.7207810
H	4.6214300	-2.3415360	-1.0250150
H	5.0263690	2.1219270	-0.6572200
H	4.0450980	2.1760370	-2.1308010
H	1.9378410	2.2776680	-0.7493850
H	2.9458540	2.3602020	0.7405200
H	2.4982380	4.9099740	0.9307190

Peroxyhemiacetal Dimer @ 373 K

C	-4.2066860	2.7807910	1.4007880
C	-4.7181900	1.3755570	1.2317020
O	-5.8218450	1.0319010	1.6935190
C	-3.8551290	0.3740610	0.5033220
C	-2.7139500	0.8102910	-0.4514670
C	-3.1028940	-0.3479510	-1.4223870
C	-4.4762840	-0.5124780	-0.6487050
C	-4.9306050	-1.9175880	-0.2554640
C	-5.5973570	0.2079370	-1.4116130
C	-2.1600650	-1.5611600	-1.5152540
C	-1.4143830	-2.0262160	-0.2564470
O	-0.2097910	-1.2336880	-0.1839930
O	0.4807080	-1.6269240	1.0768520
C	1.8920330	-1.9736010	0.7655340
O	2.3643180	-2.2856260	2.0642460
C	1.9208020	-3.2479470	-0.0600620
C	2.6002240	-0.7309500	0.2006360
C	2.5911890	-0.3765320	-1.3087870
C	3.9973370	0.2727400	-1.1365670
C	4.1721020	-0.5597430	0.1981980
C	4.7843050	0.1262570	1.4219930
C	4.9695790	-1.8370670	-0.1101130
C	4.0572920	1.8138750	-1.0874280
C	2.9308570	2.5394430	-0.3473290
O	3.1770180	3.9440730	-0.5901700
O	2.0985000	4.7100180	0.0545130
H	-3.1519400	2.7766390	1.7216690
H	-4.2329640	3.2974690	0.4251170
H	-4.8239340	3.3377610	2.1184970
H	-3.4604390	-0.2930760	1.2927150
H	-1.6960710	0.7868260	-0.0371900

H	-2.8878310	1.8001190	-0.8992920
H	-3.2754330	-0.0046520	-2.4566850
H	-4.1588620	-2.4716970	0.3010350
H	-5.8270530	-1.8633540	0.3849640
H	-5.1975950	-2.5104820	-1.1473400
H	-5.8219970	-0.3334660	-2.3462580
H	-6.5265650	0.2568720	-0.8207370
H	-5.3146470	1.2387800	-1.6839360
H	-2.7306930	-2.4266550	-1.8939180
H	-1.3963220	-1.3591980	-2.2879370
H	-1.9986390	-1.8832320	0.6678760
H	-1.1414310	-3.0928440	-0.3387510
H	2.5062080	-1.4496850	2.5544900
H	2.9522670	-3.5576220	-0.2729520
H	1.4190840	-4.0520630	0.4985980
H	1.3991910	-3.0983160	-1.0153390
H	2.1869630	0.1179640	0.7741130
H	1.7708470	0.2588960	-1.6736410
H	2.6416280	-1.2741230	-1.9434640
H	4.7284650	-0.0327380	-1.9042500
H	4.2290850	1.0261720	1.7271130
H	4.7988690	-0.5622740	2.2843440
H	5.8290210	0.4218200	1.2244760
H	6.0301400	-1.5744880	-0.2659560
H	4.9234750	-2.5599670	0.7207810
H	4.6214300	-2.3415360	-1.0250150
H	5.0263690	2.1219270	-0.6572200
H	4.0450980	2.1760370	-2.1308010
H	1.9378410	2.2776680	-0.7493850
H	2.9458540	2.3602020	0.7405200
H	2.4982380	4.9099740	0.9307190

Terpenylic Acid Dimer @ 298 K

C	-5.8647410	-1.7527280	-0.0075520
C	-5.9917440	-0.2989540	-0.5565260
O	-6.5842140	-2.5445320	-1.0600740
C	-6.6344540	-1.8626940	-2.2309590
C	-6.0104730	-0.4986630	-2.0786350
C	-6.6207720	-1.9722910	1.2942960
C	-4.4440180	-2.3095180	0.0551240
O	-7.1352120	-2.3701370	-3.2347430
C	-5.0194440	0.7465710	0.0298280
C	-3.5713210	0.6821000	-0.3932550
O	-2.7073950	0.6086870	0.6104600
O	-3.2171610	0.7477690	-1.5918370

H	-6.9967330	0.0478680	-0.2611990
H	-6.5851190	0.2581930	-2.6302380
H	-4.9988900	-0.5372420	-2.5170700
H	-7.6761020	-1.6767530	1.1918680
H	-6.5729240	-3.0276310	1.6037900
H	-6.1665150	-1.3629080	2.0910860
H	-3.8844640	-1.8372010	0.8762910
H	-4.4812550	-3.3914560	0.2541950
H	-3.8959940	-2.1502860	-0.8865030
H	-5.3731030	1.7425720	-0.2882630
H	-5.0713600	0.7204060	1.1276220
H	-1.7340600	0.6048720	0.2626730
C	2.4167740	-1.7525450	-1.7478400
C	2.5604250	-0.2966210	-1.2073480
O	3.1516360	-2.5446610	-0.7068280
C	3.2323060	-1.8584290	0.4598230
C	2.6192610	-0.4890550	0.3149530
C	3.1476170	-1.9809590	-3.0626170
C	0.9929420	-2.3041180	-1.7824680
O	3.7481190	-2.3672110	1.4554010
C	1.5777650	0.7477720	-1.7731950
C	0.1295820	0.6754140	-1.3509640
O	-0.7334440	0.7657220	-2.3551280
O	-0.2271520	0.5960370	-0.1544880
H	3.5582270	0.0465650	-1.5300070
H	3.2184310	0.2642750	0.8450590
H	1.6198790	-0.5125270	0.7803740
H	4.2044230	-1.6837170	-2.9830610
H	3.0950170	-3.0388620	-3.3626270
H	2.6772150	-1.3789240	-3.8555820
H	0.4149500	-1.8222900	-2.5856000
H	1.0215160	-3.3838560	-1.9946260
H	0.4684520	-2.1535070	-0.8266160
H	1.9250270	1.7442450	-1.4463820
H	1.6250070	0.7421220	-2.8716030
H	-1.7069980	0.7607510	-2.0084690

Terpenylic Acid Dimer @ 298 K

Symbol	X	Y	Z
C	-5.8647490	-1.7527260	-0.0075570
C	-5.9917460	-0.2989470	-0.5565170
O	-6.5842260	-2.5445170	-1.0600850
C	-6.6344650	-1.8626690	-2.2309630
C	-6.0104790	-0.4986410	-2.0786280
C	-6.6207780	-1.9722980	1.2942900

C	-4.4440280	-2.3095220	0.0551130
O	-7.1352260	-2.3701010	-3.2347520
C	-5.0194400	0.7465680	0.0298440
C	-3.5713170	0.6820940	-0.3932400
O	-2.7073910	0.6086760	0.6104740
O	-3.2171580	0.7477650	-1.5918220
H	-6.9967330	0.0478770	-0.2611850
H	-6.5851230	0.2582230	-2.6302230
H	-4.9988970	-0.5372200	-2.5170650
H	-7.6761070	-1.6767530	1.1918680
H	-6.5729350	-3.0276420	1.6037740
H	-6.1665160	-1.3629260	2.0910860
H	-3.8844700	-1.8372130	0.8762820
H	-4.4812690	-3.3914610	0.2541770
H	-3.8960050	-2.1502870	-0.8865140
H	-5.3730940	1.7425740	-0.2882380
H	-5.0713550	0.7203940	1.1276390
H	-1.7340560	0.6048600	0.2626860
C	2.4167770	-1.7525450	-1.7478460
C	2.5604280	-0.2966230	-1.2073470
O	3.1516420	-2.5446650	-0.7068400
C	3.2323140	-1.8584400	0.4598150
C	2.6192680	-0.4890650	0.3149530
C	3.1476180	-1.9809500	-3.0626260
C	0.9929450	-2.3041190	-1.7824750
O	3.7481280	-2.3672270	1.4553880
C	1.5777660	0.7477730	-1.7731860
C	0.1295840	0.6754100	-1.3509540
O	-0.7334430	0.7657250	-2.3551150
O	-0.2271490	0.5960250	-0.1544770
H	3.5582290	0.0465650	-1.5300060
H	3.2184390	0.2642610	0.8450610
H	1.6198870	-0.5125400	0.7803760
H	4.2044250	-1.6837090	-2.9830690
H	3.0950180	-3.0388510	-3.3626420
H	2.6772160	-1.3789100	-3.8555860
H	0.4149520	-1.8222870	-2.5856040
H	1.0215200	-3.3838550	-1.9946380
H	0.4684570	-2.1535120	-0.8266210
H	1.9250280	1.7442440	-1.4463680
H	1.6250070	0.7421290	-2.8715950
H	-1.7069970	0.7607500	-2.0084560

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer alkyl carboxylate @ 298 K**

C	4.3654270	0.5795860	0.9810390
C	2.9394090	0.6338310	1.5248920

C	5.3726540	0.1899590	2.0522510
O	4.7084290	1.9796810	0.5588830
C	4.5442600	-0.2048640	-0.3533330
C	4.1500300	0.8274940	-1.4186870
C	4.5516120	2.1337400	-0.7794900
C	3.9197780	-1.6150850	-0.4286280
C	2.4159010	-1.7557480	-0.4256190
O	1.8205830	-2.4385890	0.4386300
O	1.7886280	-1.1564940	-1.4271020
O	4.7284890	3.2287870	-1.3134900
H	2.8800770	1.3886960	2.3237160
H	2.2105420	0.8989200	0.7433680
H	2.6568520	-0.3362740	1.9598230
H	5.2080130	-0.8574950	2.3493310
H	6.4027870	0.2860250	1.6766870
H	5.2570400	0.8189570	2.9481600
H	5.6297990	-0.3754700	-0.4574670
H	3.0631840	0.8606220	-1.6035830
H	4.6511690	0.6943730	-2.3873310
H	4.2686600	-2.0778490	-1.3683210
H	4.3066340	-2.2274840	0.3979880
H	0.7627670	-1.3061450	-1.3719070
C	-5.3126910	1.7441760	-0.3375180
C	-3.9020070	1.2573150	-0.1932920
C	-3.4173840	0.3155030	-1.3257350
C	-3.7261200	-0.9065460	-0.4249030
C	-3.7514750	0.0360470	0.8330530
C	-2.8894040	-2.2011590	-0.4603080
C	-1.3895060	-2.0600150	-0.4638100
C	-2.4148480	0.1575400	1.5723140
C	-4.8880660	-0.2126110	1.8232730
O	-6.1727860	1.2776580	-1.0903340
O	-5.5837500	2.7791200	0.5020710
O	-0.7670010	-2.6689850	0.5383730
O	-0.7764370	-1.4511080	-1.3715520
H	-3.2562840	2.1127100	0.0537230
H	-2.3436930	0.4548080	-1.5089980
H	-3.9591020	0.3757590	-2.2811980
H	-4.7654590	-1.2236290	-0.6131960
H	-3.1843470	-2.8568540	0.3724880
H	-3.1348670	-2.7322890	-1.3974050
H	-1.5736900	0.3586340	0.8897470
H	-2.4581850	0.9866790	2.2979970
H	-2.1931350	-0.7648360	2.1335480
H	-4.7264440	-1.1686010	2.3497420
H	-4.9374670	0.5818410	2.5866160

H	-5.8680150	-0.2720480	1.3221490
H	-6.5287890	3.0277890	0.3879060
H	0.2573050	-2.5623710	0.4595850

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer alkyl carboxylate @ 373 K**

C	4.3654270	0.5795860	0.9810390
C	2.9394090	0.6338310	1.5248920
C	5.3726540	0.1899590	2.0522510
O	4.7084290	1.9796810	0.5588830
C	4.5442600	-0.2048640	-0.3533330
C	4.1500300	0.8274940	-1.4186870
C	4.5516120	2.1337400	-0.7794900
C	3.9197780	-1.6150850	-0.4286280
C	2.4159010	-1.7557480	-0.4256190
O	1.8205830	-2.4385890	0.4386300
O	1.7886280	-1.1564940	-1.4271020
O	4.7284890	3.2287870	-1.3134900
H	2.8800770	1.3886960	2.3237160
H	2.2105420	0.8989200	0.7433680
H	2.6568520	-0.3362740	1.9598230
H	5.2080130	-0.8574950	2.3493310
H	6.4027870	0.2860250	1.6766870
H	5.2570400	0.8189570	2.9481600
H	5.6297990	-0.3754700	-0.4574670
H	3.0631840	0.8606220	-1.6035830
H	4.6511690	0.6943730	-2.3873310
H	4.2686600	-2.0778490	-1.3683210
H	4.3066340	-2.2274840	0.3979880
H	0.7627670	-1.3061450	-1.3719070
C	-5.3126910	1.7441760	-0.3375180
C	-3.9020070	1.2573150	-0.1932920
C	-3.4173840	0.3155030	-1.3257350
C	-3.7261200	-0.9065460	-0.4249030
C	-3.7514750	0.0360470	0.8330530
C	-2.8894040	-2.2011590	-0.4603080
C	-1.3895060	-2.0600150	-0.4638100
C	-2.4148480	0.1575400	1.5723140
C	-4.8880660	-0.2126110	1.8232730
O	-6.1727860	1.2776580	-1.0903340
O	-5.5837500	2.7791200	0.5020710
O	-0.7670010	-2.6689850	0.5383730
O	-0.7764370	-1.4511080	-1.3715520
H	-3.2562840	2.1127100	0.0537230
H	-2.3436930	0.4548080	-1.5089980
H	-3.9591020	0.3757590	-2.2811980
H	-4.7654590	-1.2236290	-0.6131960

H	-3.1843470	-2.8568540	0.3724880
H	-3.1348670	-2.7322890	-1.3974050
H	-1.5736900	0.3586340	0.8897470
H	-2.4581850	0.9866790	2.2979970
H	-2.1931350	-0.7648360	2.1335480
H	-4.7264440	-1.1686010	2.3497420
H	-4.9374670	0.5818410	2.5866160
H	-5.8680150	-0.2720480	1.3221490
H	-6.5287890	3.0277890	0.3879060
H	0.2573050	-2.5623710	0.4595850

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer carboxylate @ 298 K**

C	-1.4235620	-1.3537380	-0.4731970
C	-2.9058920	-1.2902300	-0.2761030
C	-3.6832260	-0.4549710	-1.3273350
C	-3.7029650	0.7443560	-0.3471920
C	-3.3536250	-0.2263510	0.8387670
C	-4.8791150	1.7348250	-0.2680310
C	-6.2729540	1.1587390	-0.2325340
C	-4.5650340	-0.7740470	1.6003020
C	-2.2953460	0.2796610	1.8182370
O	-0.7887920	-0.5501660	-1.1963870
O	-0.8270130	-2.3216070	0.2178610
O	-7.0051350	1.6167910	0.8157120
O	-6.7524410	0.3939700	-1.0732620
H	-3.2749920	-2.3064180	-0.0758330
H	-4.6791950	-0.8837910	-1.5003900
H	-3.1837720	-0.2950990	-2.2941710
H	-2.8094160	1.3625970	-0.5356060
H	-4.7404270	2.4079190	0.5911980
H	-4.8529600	2.3634720	-1.1765860
H	-5.3381820	-1.1792810	0.9286840
H	-4.2504700	-1.5890600	2.2731210
H	-5.0243530	0.0121660	2.2219160
H	-2.7080070	1.1080810	2.4185690
H	-1.9824130	-0.5133910	2.5178600
H	-1.3989670	0.6604770	1.3022230
H	0.1956590	-2.2926270	0.0897030
H	-7.9099500	1.2354970	0.7477080
C	4.8356380	0.1496140	0.9174040
C	3.5039320	0.2432400	1.6589270
C	5.8794680	-0.6218340	1.7110890
O	5.3474940	1.5555860	0.7888610
C	4.7422700	-0.2918110	-0.5743600
C	4.4140470	1.0172690	-1.3060330
C	5.0794640	2.0588230	-0.4414880

C	3.8905090	-1.5416820	-0.8812830
C	2.3890010	-1.4818930	-0.7224430
O	1.7679230	-2.3160540	-0.0255120
O	1.7822030	-0.5342600	-1.4216340
O	5.3698850	3.2213530	-0.7240240
H	3.6517330	0.7636380	2.6176580
H	2.7479460	0.7962180	1.0803060
H	3.1163490	-0.7624050	1.8803710
H	5.5766340	-1.6775910	1.7898140
H	6.8614530	-0.5783240	1.2159790
H	5.9755160	-0.2191040	2.7310890
H	5.7680040	-0.5754320	-0.8667610
H	3.3336590	1.2371990	-1.3283320
H	4.7876530	1.0670070	-2.3381310
H	4.0673960	-1.8064780	-1.9389770
H	4.2499140	-2.3847660	-0.2745400
H	0.7525560	-0.5752330	-1.2981490

***cis*-Pinic Acid-Terpenylic Acid non-covalent Dimer carboxylate @ 373 K**

C	-1.4235620	-1.3537380	-0.4731970
C	-2.9058920	-1.2902300	-0.2761030
C	-3.6832260	-0.4549710	-1.3273350
C	-3.7029650	0.7443560	-0.3471920
C	-3.3536250	-0.2263510	0.8387670
C	-4.8791150	1.7348250	-0.2680310
C	-6.2729540	1.1587390	-0.2325340
C	-4.5650340	-0.7740470	1.6003020
C	-2.2953460	0.2796610	1.8182370
O	-0.7887920	-0.5501660	-1.1963870
O	-0.8270130	-2.3216070	0.2178610
O	-7.0051350	1.6167910	0.8157120
O	-6.7524410	0.3939700	-1.0732620
H	-3.2749920	-2.3064180	-0.0758330
H	-4.6791950	-0.8837910	-1.5003900
H	-3.1837720	-0.2950990	-2.2941710
H	-2.8094160	1.3625970	-0.5356060
H	-4.7404270	2.4079190	0.5911980
H	-4.8529600	2.3634720	-1.1765860
H	-5.3381820	-1.1792810	0.9286840
H	-4.2504700	-1.5890600	2.2731210
H	-5.0243530	0.0121660	2.2219160
H	-2.7080070	1.1080810	2.4185690
H	-1.9824130	-0.5133910	2.5178600
H	-1.3989670	0.6604770	1.3022230
H	0.1956590	-2.2926270	0.0897030
H	-7.9099500	1.2354970	0.7477080

C	4.8356380	0.1496140	0.9174040
C	3.5039320	0.2432400	1.6589270
C	5.8794680	-0.6218340	1.7110890
O	5.3474940	1.5555860	0.7888610
C	4.7422700	-0.2918110	-0.5743600
C	4.4140470	1.0172690	-1.3060330
C	5.0794640	2.0588230	-0.4414880
C	3.8905090	-1.5416820	-0.8812830
C	2.3890010	-1.4818930	-0.7224430
O	1.7679230	-2.3160540	-0.0255120
O	1.7822030	-0.5342600	-1.4216340
O	5.3698850	3.2213530	-0.7240240
H	3.6517330	0.7636380	2.6176580
H	2.7479460	0.7962180	1.0803060
H	3.1163490	-0.7624050	1.8803710
H	5.5766340	-1.6775910	1.7898140
H	6.8614530	-0.5783240	1.2159790
H	5.9755160	-0.2191040	2.7310890
H	5.7680040	-0.5754320	-0.8667610
H	3.3336590	1.2371990	-1.3283320
H	4.7876530	1.0670070	-2.3381310
H	4.0673960	-1.8064780	-1.9389770
H	4.2499140	-2.3847660	-0.2745400
H	0.7525560	-0.5752330	-1.2981490