Chemical Equilibrium of Zinc-Acetate Complexes in Ethanol Solution. A Theoretical Description Through Thermodynamic Cycles

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Supporting Information

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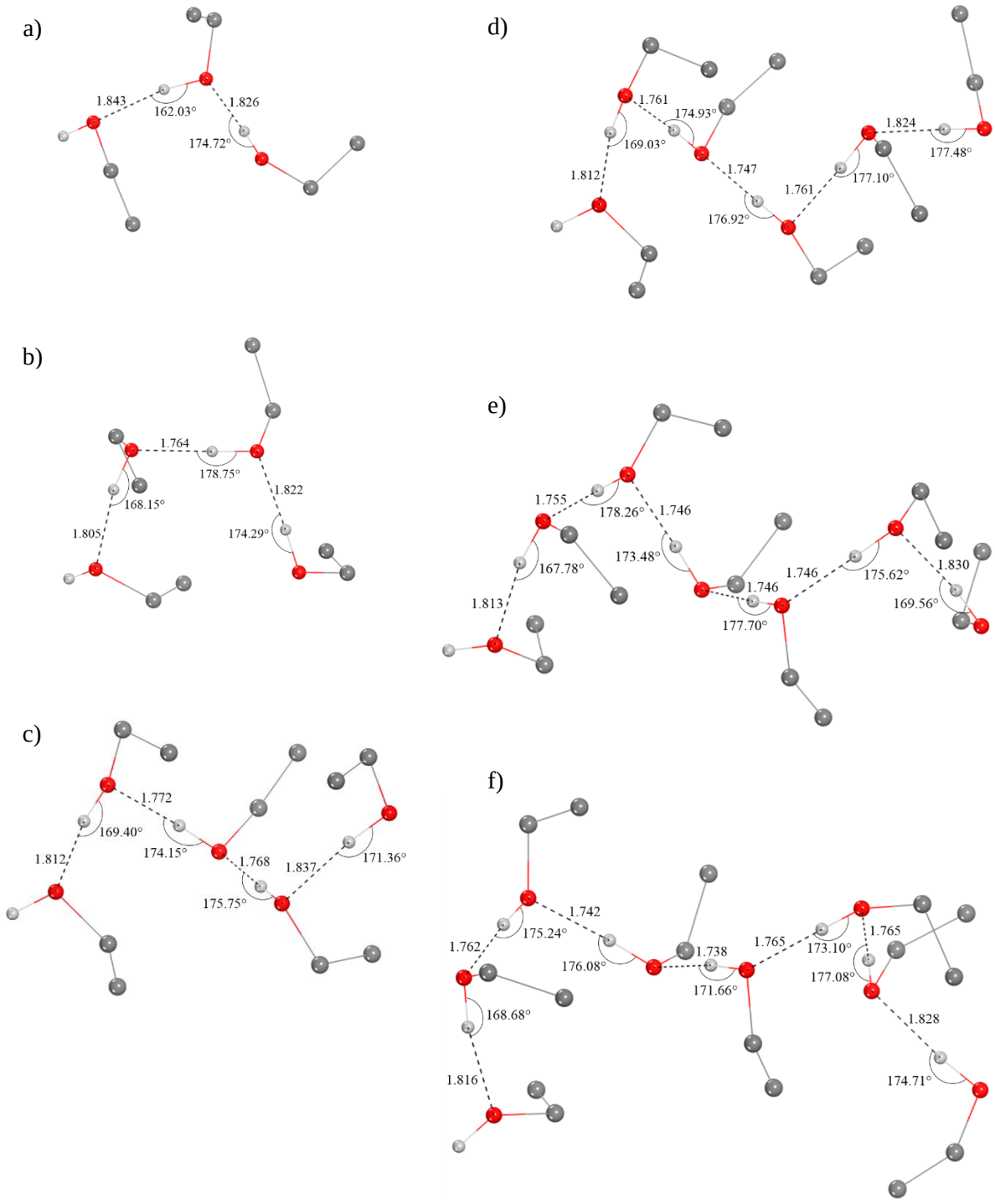


Figure S1. Relevant parameters of optimized geometries in the gas phase optimized for *linear*-gauche ethanol clusters: a) trimer, b) tetramer, c) pentamer, d) hexamer, e) heptamer and f) octamer, at the level M05-2X/6-31+G(d)

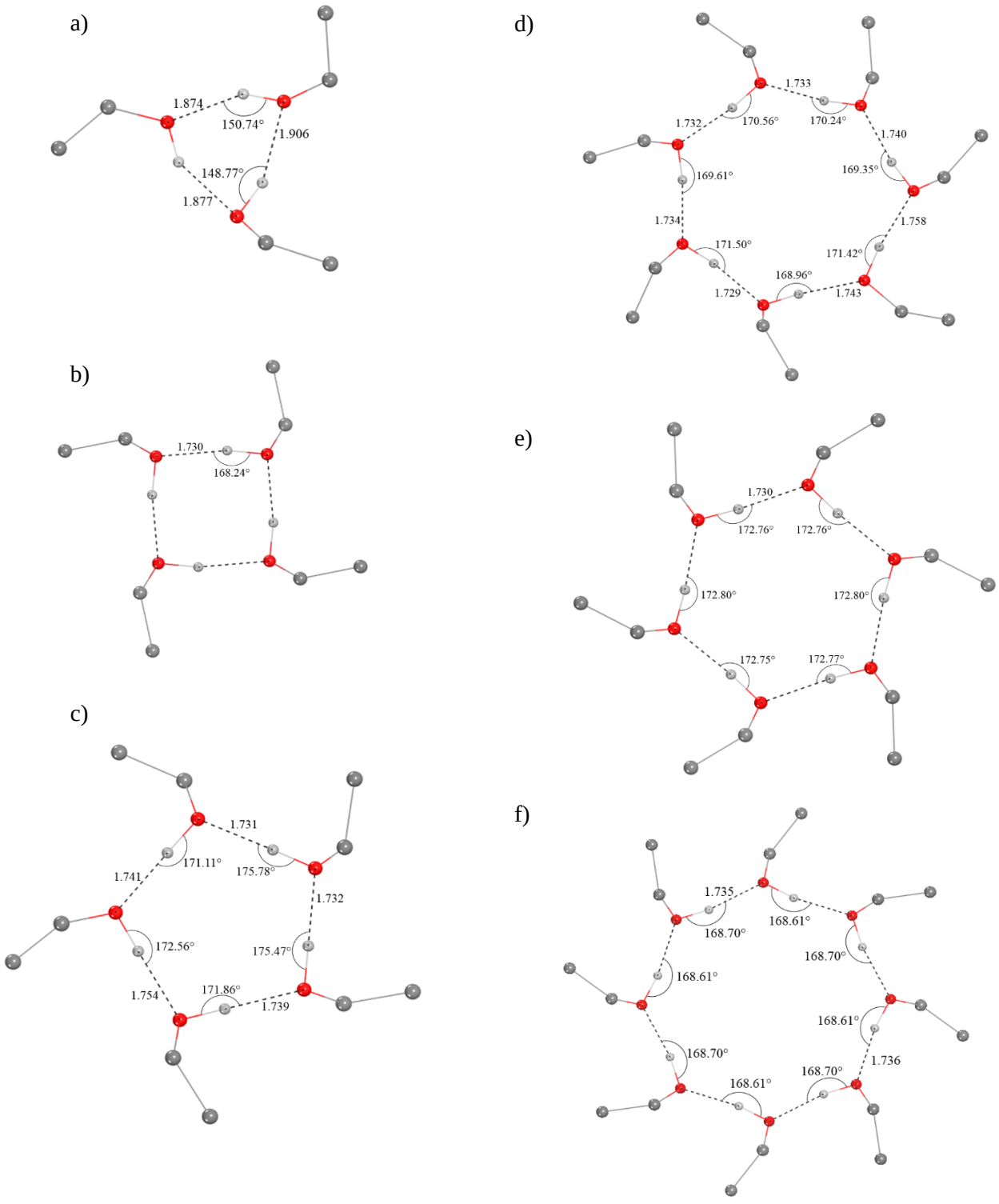


Figure S2. Relevant parameters of optimized geometries in the gas phase optimized for cyclic-gauche ethanol clusters: a) trimer, b) tetramer, c) pentamer, d) hexamer, e) heptamer and f) octamer, at the level M05-2X/6-31+G(d)

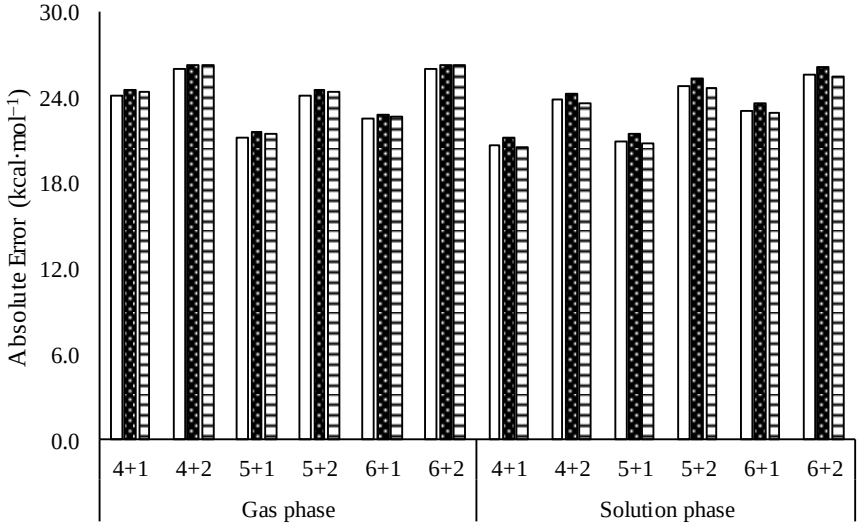
Table S1. Thermodynamic stability of ethanol clusters by comparing their corresponding solvation Gibbs free energies $\left(\Delta G^{*}_{\mathrm{solv}}\left(\mathrm{EtOH}\right)_{\mathrm{x}}\right)$ as well as their relative solution phase Gibbs free energies $\left(\Delta G_{\mathrm{s}}\left(\mathrm{EtOH}\right)_{x}\right)$.

x	$\Delta G^{*}_{\mathrm{solv}}\left(\mathrm{EtOH}\right)_{x}$	$\Delta G_{\mathrm{s}}\left(\mathrm{EtOH}\right)_{x}^{linear} - \Delta G_{\mathrm{s}}\left(\mathrm{EtOH}\right)_{x}^{cyclic}$
	Cyclic-*gauche*	
3	-10.27	1.03
4	-11.17	3.16
5	-12.71	4.12
6	-13.62	4.62
7	-15.54	5.42
8	-16.84	5.45
	Linear-*gauche*	
3	-12.86	
4	-14.08	
5	-17.64	
6	-19.98	
7	-21.65	
8	-24.44	

Table S2. Average O-C-O bond distances obtained for the $\left[\mathrm{OAc}\left(\mathrm{EtOH}\right)_{j_{\mathrm{first}}}\right]^{-}\left(\mathrm{EtOH}\right)_{j_{\mathrm{second}}}$ species at the M052X/6-31+G (d) level of theory with the SMD continuum solvation model.

Species	Ethanol		Water[46]
	Gas phase	Solution phase	
Acetate	1.256	1.264	
$\left[\mathrm{Ac}\left(\mathrm{EtOH}\right)\right]^{-}$	1.267, 1.249	1.271, 1.258	1.265
$\left[\mathrm{Ac}\left(\mathrm{EtOH}\right)_{2}\right]^{-}$	1.278, 1.241	1.278, 1.253	1.258, 1.270
$\left[\mathrm{Ac}\left(\mathrm{EtOH}\right)_{3}\right]^{-}$	1.274, 1.248	1.272, 1.259	1.259, 1.273
$\left[\mathrm{Ac}\left(\mathrm{EtOH}\right)_{4}\right]^{-}$	1.261, 1.262	1.267, 1.265	1.260, 1.272
$\left[\mathrm{Ac}\left(\mathrm{EtOH}\right)_{4}\right]^{-}\left(\mathrm{EtOH}\right)$	1.265, 1.259	1.266	1.262, 1.274
$\left[\mathrm{Ac}\left(\mathrm{EtOH}\right)_{4}\right]^{-}\left(\mathrm{EtOH}\right)_{2}$	1.261, 1.262	1.267, 1.265	1.259, 1.278

a)



b)

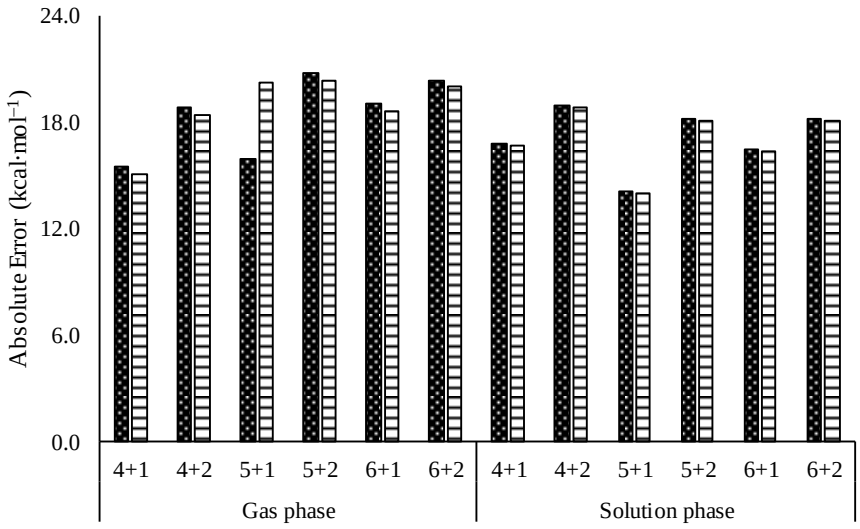
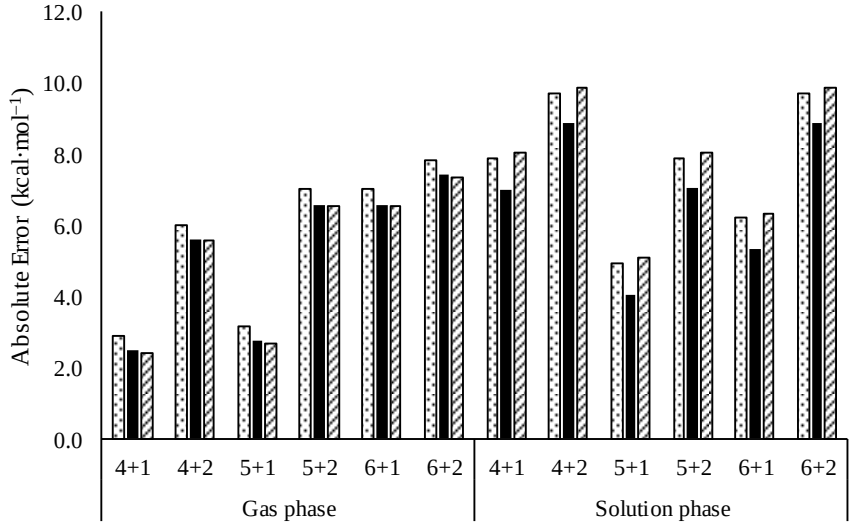


Figure S3. Absolute errors in the computation of $\Delta_r G^*_{s,1}$ for the $\left[\mathrm{Zn(OAc)}\right]^+$ species at the M05-2X/6-31+G(d) /SMD level of theory; by means of a) *variant 1* (Eq.(7)) and b) *variant 2* (Eq.(11)), for $j=1$ (white solid bars) $j=2$ (white dotted bars) $j=3$ (bars with horizontal lines)

a)



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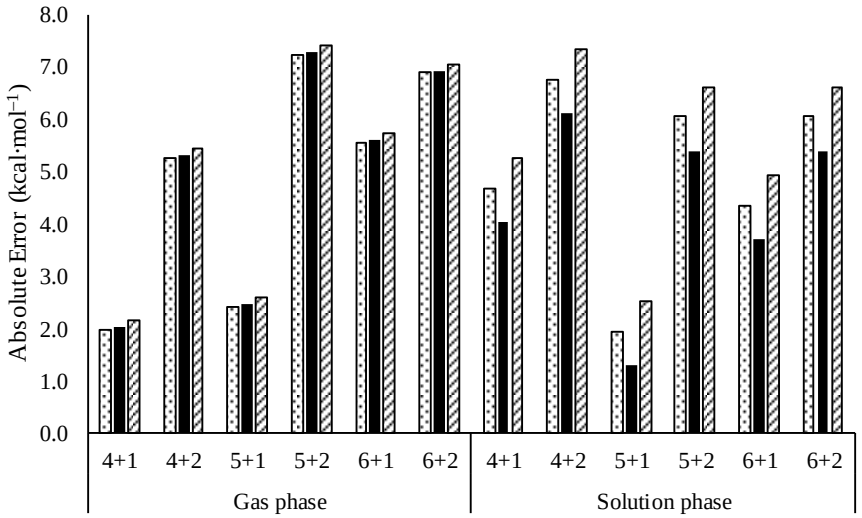
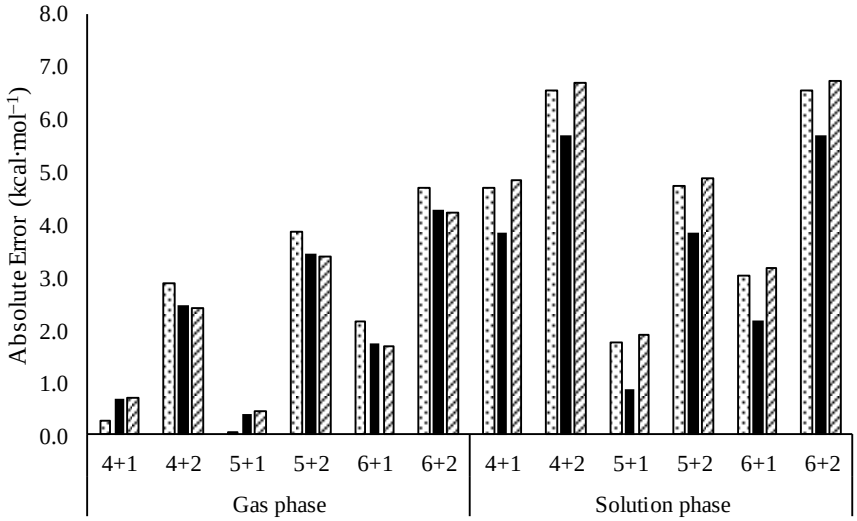


Figure S4. Absolute errors in the computation of $\Delta_r G^*_{s,1}$ for the $\left[\mathrm{Zn(OAc)(EtOH)_2}\right]^+$ species at the M05-2X/6-31+G(d) /SMD level of theory; by means of a) *variant 1* (Eq.(7)) and b) *variant 2* (Eq.(11)), for $j = 4+0$ (dotted bars) $j = 4+1$(solid bars) and $j = 4+2$ (bars with diagonal lines).

a)



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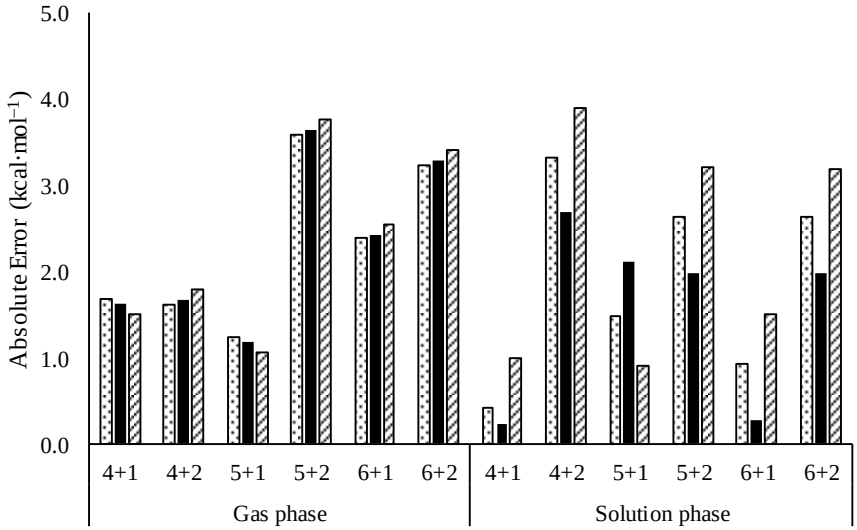
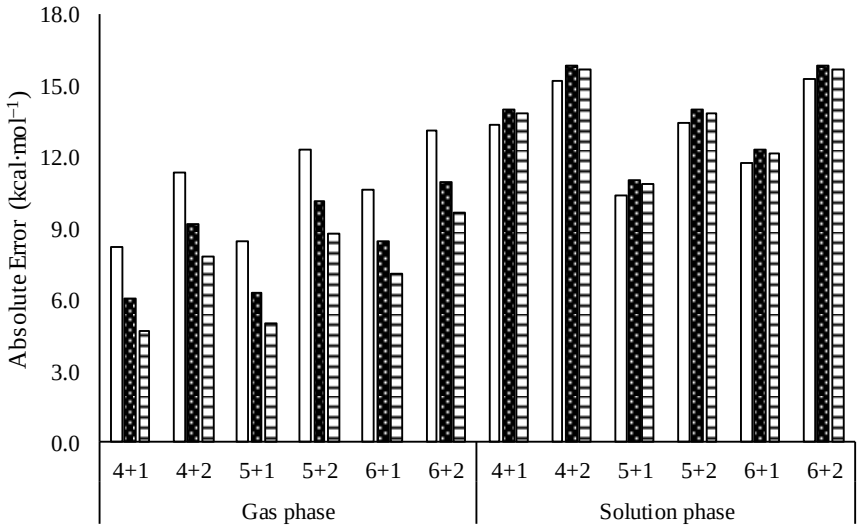


Figure S5. Absolute errors in the computation of $\Delta_r G^*_{s,1}$ for the $\left[\mathrm{Zn(OAc)(EtOH)_2}\right]^+(\mathrm{EtOH})$ species at the M05-2X/6-31+G(d)/SMD level of theory; by means of a) *variant 1* (Eq.(7)) and b) *variant 2* (Eq.(11)), for $j = 4+0$ (dotted bars) $j = 4+1$ (solid bars) and $j = 4+2$ (bars with diagonal lines).

a)



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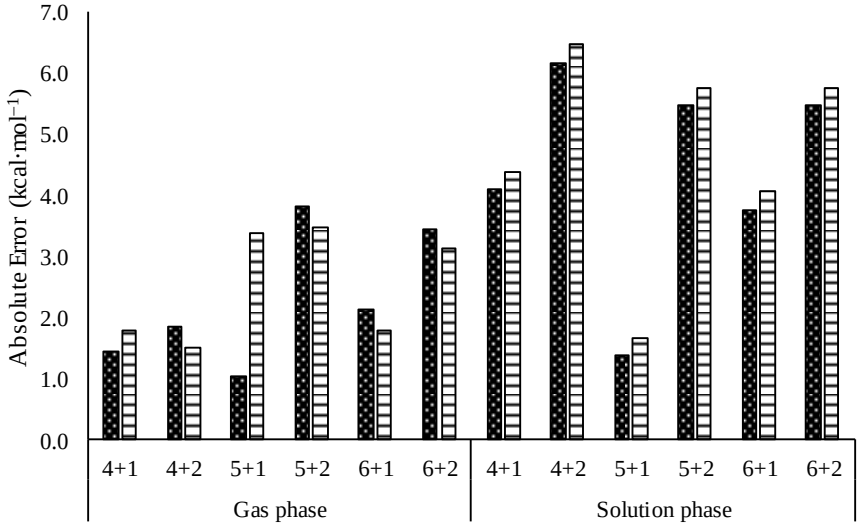
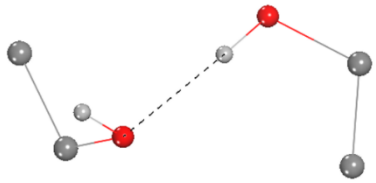


Figure S6. Absolute errors in the computation of $\Delta_r G^*_{s,2}$ for the $\left[\mathrm{Zn(OAc)_2}\right]$ species at the M05-2X/6-31+G(d)/SMD level of theory; by means of a) *variant 1* (Eq.(7)) and b) *variant 2* (Eq. (11)), for $j=1$ (white solid bars) $j=2$ (white dotted bars) $j=3$ (bars with horizontal lines).

Optimized geometries of Zinc complexes in gas phase at the M05-2X/6-31+G(d) level of theory.

Gauche-$(EtOH)_2$



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H, 3.158841, -1.353165, -0.618326
H, 1.47967, -1.562175, -0.096173
H, 1.836082, -0.695328, -1.602111
H, 2.93316, 1.130914, -0.301691
H, 2.609674, 0.267176, 1.203277
H, 0.344395, 0.517285, 0.652964
C, -2.385505, 0.715011, -0.569761
C, -1.794527, -0.650249, -0.264053
O, -1.097635, -0.664561, 0.990247
H, -2.879983, 0.703581, -1.543752
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H, -1.597917, 1.469683, -0.584947
H, -1.042235, -0.917718, -1.004461
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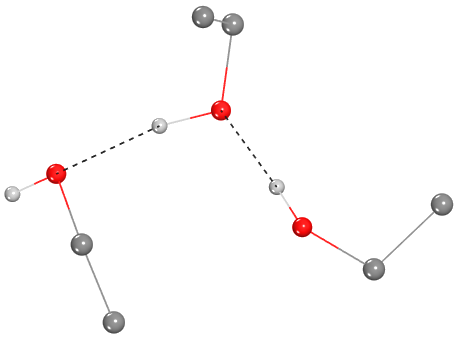
Linear-*gauche* $(EtOH)_3$



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H, -3.259674, -0.260852, -0.943689
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H, -1.391782, -0.636899, 1.152171
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O, -0.054874, 1.025234, -0.977267
C, 0.126277, 2.34621, -0.463848
C, -0.330623, 2.460656, 0.982767
H, -0.406473, 3.060991, -1.09811
H, 1.193464, 2.551804, -0.5493
H, 0.222374, 1.759082, 1.610523
H, -1.397013, 2.237229, 1.064837
H, -0.162377, 3.473364, 1.357512
H, 0.801693, -0.152366, 0.12431
O, 1.194228, -0.768406, 0.773488
C, 2.296048, -1.415293, 0.158003
C, 3.341392, -0.419736, -0.326122
H, 1.95487, -2.038023, -0.678671
H, 2.720712, -2.078176, 0.912565
H, 3.693799, 0.188564, 0.5091
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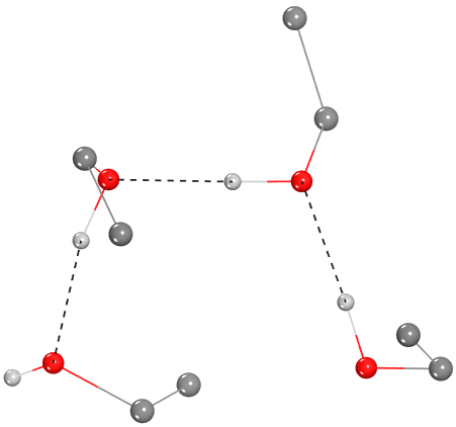
Linear-*gauche* $(EtOH)_4$



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C, 2.20786, -0.838054, 1.649213
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H, 3.265556, -0.688279, 1.883472
H, 1.959047, -1.877989, 1.862198
H, 0.279931, -0.055852, 2.223864
H, 1.58618, 1.144366, 2.242161
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O, -0.596801, -1.309054, -0.361558
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H, 1.18534, -3.323175, -0.711483
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O, -2.117343, 1.034948, -0.47528
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H, -2.308662, 1.318987, 2.194124
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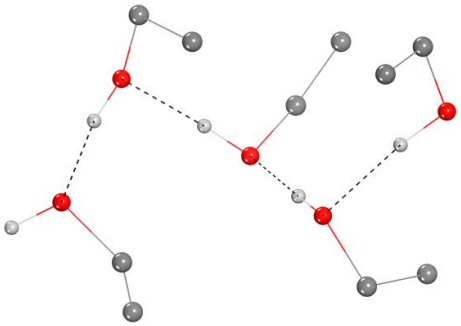
Linear-*gauche* $(\mathrm{EtOH})_5$



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O, -0.599098, 0.809528, 1.703178
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C, 1.255268, -0.471309, 2.659576
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H, 0.649129, 1.551075, 3.112581
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C, 2.625256, -1.846549, -2.209419
H, 2.511813, -2.113135, -0.066762
H, 4.155004, -1.949598, -0.688206
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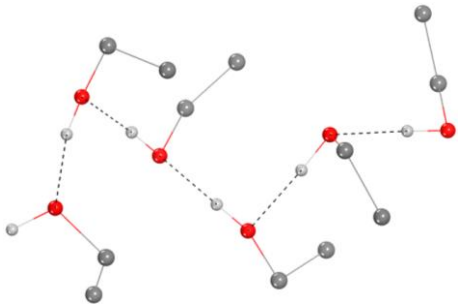
Linear-*gauche* $(EtOH)_6$



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C, -1.614017, 1.393443, -2.41019
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O, -4.096548, 0.537249, 0.176455
C, -4.368399, -0.733161, -0.389444
C, -4.255908, -1.853666, 0.635888
H, -3.694668, -0.928988, -1.234631
H, -5.383035, -0.680064, -0.785973
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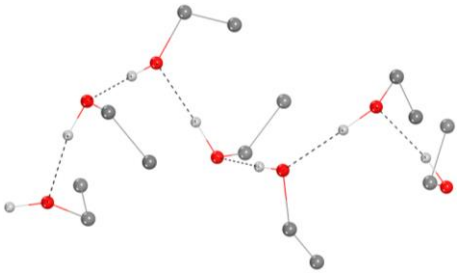
Linear-*gauche* $(EtOH)_7$



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O, 4.036361, -1.16631, -0.533185
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O, 2.13207, 0.124064, -2.018701
C, 1.534607, -0.794995, -2.935204
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H, 0.078964, -2.390233, -2.981057
H, 1.141731, 0.969582, -0.856175
O, 0.616151, 1.370779, -0.124739
C, -0.217216, 2.404571, -0.650536
C, -1.130848, 1.900073, -1.756155
H, 0.410962, 3.224594, -1.012995
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H, -1.750422, 1.073669, -1.402565
H, -0.542727, 1.55398, -2.610059
H, -1.788585, 2.702184, -2.101091
H, -0.151986, 0.011808, 0.658326
O, -0.587138, -0.772414, 1.064645
C, -0.698149, -0.562979, 2.47271
C, -1.498581, 0.686842, 2.803147
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H, -1.189186, -1.451123, 2.871489
H, -2.504885, 0.624752, 2.383465
H, -1.000249, 1.572837, 2.400734
H, -1.582179, 0.809344, 3.8861
H, -2.045311, -0.99651, 0.130666
O, -2.851795, -1.057422, -0.429569
C, -3.161576, -2.431469, -0.642207
C, -3.445602, -3.153317, 0.666615
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H, -4.039045, -2.446244, -1.289045
H, -4.26282, -2.662734, 1.199309
H, -2.559339, -3.143438, 1.305895
H, -3.721916, -4.194526, 0.4824
H, -4.113975, -0.093215, 0.4783
O, -4.666131, 0.551071, 0.961882
C, -4.477748, 1.8122, 0.344606
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H, -3.417867, 2.100028, 0.379079
H, -5.033921, 2.53382, 0.944535
H, -6.032639, 1.568564, -1.128257
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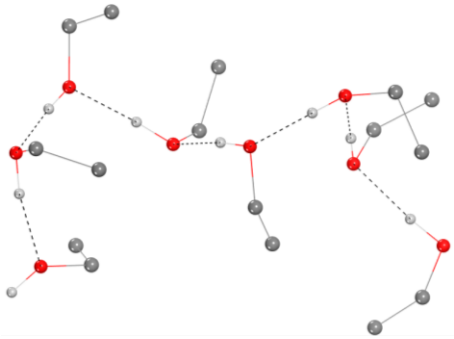
Linear-*gauche* $(EtOH)_8$



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O, -4.103169, -2.837575, -0.406882
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C, -2.768749, -2.15613, -2.347668
H, -2.32857, -1.87598, -0.262317
H, -2.200524, -3.559726, -0.793429
H, -3.316018, -1.216154, -2.439266
H, -3.224465, -2.898531, -3.009666
H, -1.742643, -1.988037, -2.680376
H, -4.917721, -1.272186, 0.022936
O, -5.178541, -0.371685, 0.301751
C, -5.12903, -0.301996, 1.728028
C, -3.746198, -0.631083, 2.267726
H, -5.879107, -0.977291, 2.149216
H, -5.417546, 0.716992, 1.986575
H, -2.99322, 0.034599, 1.839432
H, -3.482414, -1.662779, 2.02391
H, -3.722093, -0.520879, 3.354668
H, -4.237935, 0.770363, -0.654804
O, -3.654616, 1.350764, -1.193404
C, -3.902771, 2.714791, -0.854401
C, -3.332773, 3.075922, 0.509234
H, -4.978816, 2.906312, -0.890192
H, -3.43336, 3.311762, -1.636713
H, -2.260495, 2.871341, 0.543406
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H, -3.491269, 4.135794, 0.723216
H, -2.038471, 0.731856, -0.989964
O, -1.152576, 0.322769, -0.858854
C, -0.27229, 0.759559, -1.899215
C, -0.000103, 2.253379, -1.816248
H, -0.710091, 0.499148, -2.867878
H, 0.653735, 0.197692, -1.775618
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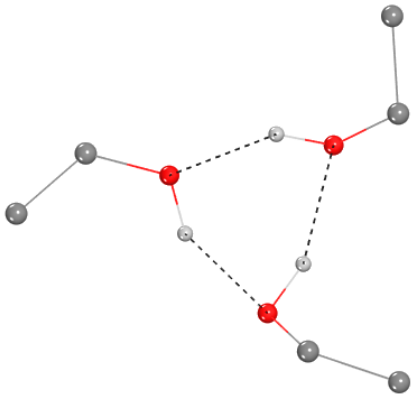
H, -0.931701, 2.819032, -1.900514
H, 0.658384, 2.565106, -2.630776
H, -0.508084, 0.401177, 0.753044
O, -0.051928, 0.343501, 1.623817

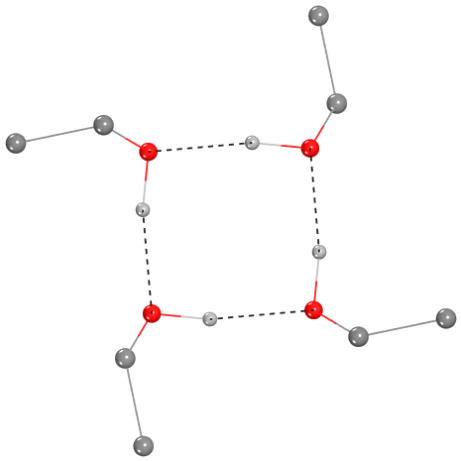
C, 0.134724, -1.0371, 1.933089
C, 0.939921, -1.758216, 0.862488
H, -0.8407, -1.514985, 2.070578
H, 0.652141, -1.065154, 2.892699
H, 1.90072, -1.264057, 0.708092
H, 0.402322, -1.754616, -0.088551
H, 1.124976, -2.796149, 1.152647
H, 1.412926, 1.291139, 1.356962
O, 2.221871, 1.786412, 1.094718
C, 3.068884, 1.942638, 2.23349
C, 3.718144, 0.631414, 2.650019
H, 2.489217, 2.3695, 3.056992
H, 3.829139, 2.670215, 1.948373
H, 4.321614, 0.219761, 1.838226
H, 2.956504, -0.102671, 2.926115
H, 4.366909, 0.786616, 3.516076
H, 2.86598, 0.914872, -0.298935
O, 3.208443, 0.386689, -1.054726
C, 3.866477, 1.264002, -1.967755
C, 4.965444, 2.067611, -1.288472
H, 3.131688, 1.931258, -2.42973
H, 4.282556, 0.626413, -2.748216
H, 5.692722, 1.397655, -0.825663
H, 4.540621, 2.713101, -0.515855
H, 5.482685, 2.700186, -2.014191
H, 4.512744, -0.742011, -0.449629
O, 5.265095, -1.274246, -0.124377
C, 4.770903, -2.524459, 0.322148
C, 4.041729, -3.279779, -0.781232
H, 4.108033, -2.388824, 1.18706
H, 5.638682, -3.091535, 0.661129
H, 4.713593, -3.45006, -1.624491
H, 3.185092, -2.701427, -1.136829
H, 3.679066, -4.245873, -0.419195

Cyclic-*gauche* $(\mathrm{EtOH})_3$



C, 2.095805, -2.706209, 0.139158
C, 0.688166, -2.230515, 0.458688
O, 0.062172, -1.639839, -0.679265
H, 0.614877, -0.881661, -0.954946
H, 2.074052, -3.420317, -0.685322
H, 2.728214, -1.86304, -0.151435
H, 2.54819, -3.186106, 1.010211
H, 0.053415, -3.06742, 0.748418
H, 0.704896, -1.514169, 1.288518
H, -1.21066, -0.411186, -0.053014
O, -1.453489, 0.487729, 0.248858
C, -2.745455, 0.827798, -0.248865
C, -3.816687, -0.102475, 0.296473
H, -2.740623, 0.810551, -1.343384
H, -2.927359, 1.853079, 0.072029
H, -3.818153, -0.075892, 1.387215
H, -3.632476, -1.130628, -0.024672
H, -4.804421, 0.193824, -0.064584
H, 0.198021, 1.124274, -0.368335
O, 1.08332, 0.954031, -0.747807
C, 2.081524, 1.441485, 0.143483
C, 1.988253, 2.948422, 0.320535
H, 3.038236, 1.166545, -0.300673
H, 1.999699, 0.936867, 1.112867
H, 1.029523, 3.223137, 0.76711
H, 2.074507, 3.445587, -0.646709
H, 2.784401, 3.310169, 0.97559

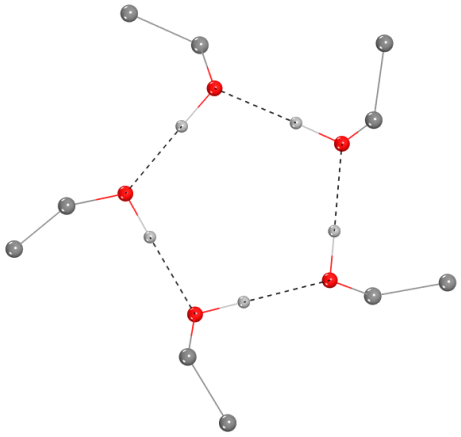
Cyclic-*gauche* $(\mathrm{EtOH})_4$



C, -3.911302, -0.161345, 0.963906
C, -2.693351, 0.731903, 1.13299
O, -1.821066, 0.636151, 0.008141
H, -1.500496, -0.293198, -0.056914
H, -4.45126, 0.106496, 0.054292
H, -3.605597, -1.207894, 0.892438
H, -4.585948, -0.059733, 1.817362
H, -2.987546, 1.779558, 1.19985

H, -2.15066, 0.471383, 2.047313
H, -0.293196, 1.500511, 0.056924
O, 0.636153, 1.821055, -0.008248
C, 0.731878, 2.692979, -1.13338
C, -0.161296, 3.911029, -0.964622
H, 0.471269, 2.150012, -2.047514
H, 1.779544, 2.987099, -1.200402
H, 0.10663, 4.451257, -0.055193
H, -1.207855, 3.605398, -0.892993
H, -0.059705, 4.585407, -1.818293
H, 1.500485, 0.293173, -0.056763
O, 1.821048, -0.636165, 0.008497
C, 2.69319, -0.731717, 1.133474
C, 3.911171, 0.161487, 0.964376
H, 2.987366, -1.779362, 1.200567
H, 2.150387, -0.47102, 2.04768
H, 3.605486, 1.208026, 0.892677
H, 4.45124, -0.106528, 0.054879
H, 4.585711, 0.060026, 1.817935
H, 0.29317, -1.500515, 0.057224
O, -0.636168, -1.821075, -0.008031
C, -0.73173, -2.693156, -1.133056
C, 0.161469, -3.911151, -0.964027
H, -0.471032, -2.150304, -2.047233
H, -1.779377, -2.987322, -1.200161
H, -0.106545, -4.451267, -0.054559
H, 1.208008, -3.605471, -0.892314
H, 0.060004, -4.585645, -1.817621

Cyclic-*gauche* $(\mathrm{EtOH})_5$



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O, 2.258172, -0.138073, -0.181015
H, 1.756726, 0.701256, -0.305339
H, 4.723198, 0.512836, -1.031664
H, 3.947763, 1.964364, -0.384239
H, 5.278234, 1.203661, 0.507929
H, 3.839179, -0.830564, 0.874902
H, 3.08813, 0.612719, 1.561848
H, 1.193523, -1.484972, 0.107741
O, 0.570391, -2.247434, 0.119786
C, 0.882143, -3.084682, -0.993748
C, 2.279649, -3.668994, -0.87107
H, 0.784914, -2.515694, -1.923362
H, 0.130457, -3.874887, -0.9986
H, 2.372935, -4.230539, 0.060047
H, 3.023368, -2.868974, -0.874307
H, 2.492386, -4.33766, -1.708686
H, -1.038704, -1.609933, 0.095811
O, -1.946719, -1.228278, 0.151944
C, -2.556067, -1.707948, 1.349378
C, -2.726094, -3.217927, 1.313997
H, -3.523996, -1.210088, 1.419133
H, -1.957748, -1.409246, 2.215765
H, -1.750947, -3.705059, 1.243541
H, -3.325184, -3.508727, 0.449356
H, -3.221896, -3.57183, 2.221198
H, -1.844972, 0.488386, -0.056961
O, -1.782031, 1.452943, -0.252725
C, -2.628858, 1.740226, -1.364342
C, -4.083193, 1.43707, -1.043042
H, -2.301715, 1.168108, -2.237973
H, -2.493045, 2.799998, -1.583431
H, -4.403846, 2.010733, -0.171695
H, -4.207322, 0.373577, -0.826899
H, -4.726239, 1.692336, -1.888833
H, -0.112787, 1.925273, -0.372886
O, 0.83342, 2.192849, -0.301053
C, 0.953994, 3.030061, 0.847591
C, 0.137327, 4.302747, 0.692941
H, 2.015136, 3.264226, 0.945815
H, 0.641276, 2.481645, 1.742528
H, -0.922947, 4.059152, 0.597975
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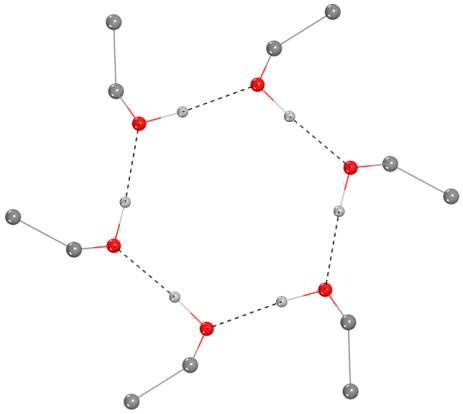
H, 0.265048, 4.950921, 1.563416

Cyclic-*gauche* $(EtOH)_6$



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H, 2.320457, -0.099122, 0.034463
H, 5.241396, 0.650261, -0.090605
H, 4.581627, -0.840335, -0.791981
H, 5.419052, 0.327526, -1.827778
H, 3.589708, 1.993421, -1.410259
H, 2.933314, 0.504581, -2.102909
H, 1.245383, 1.959063, -0.034422
O, 0.550926, 2.646757, 0.094306
C, 0.910883, 3.434645, 1.22769
C, 2.182036, 4.226891, 0.969003
H, 1.0318, 2.790284, 2.103695
H, 0.068952, 4.103118, 1.413267
H, 2.055583, 4.865198, 0.092665
H, 3.018546, 3.547995, 0.790263
H, 2.426656, 4.854916, 1.829256
H, -1.074899, 2.058116, 0.036149
O, -2.017981, 1.80126, -0.092073
C, -2.519855, 2.506429, -1.225993
C, -2.569087, 4.003541, -0.968101
H, -3.520035, 2.112167, -1.411394
H, -1.901554, 2.287955, -2.101898
H, -1.56246, 4.387587, -0.789704
H, -3.184751, 4.214115, -0.091731
H, -2.990338, 4.529399, -1.828476
H, -2.320518, 0.098944, -0.034518
O, -2.5689, -0.846493, 0.092854
C, -3.431645, -0.930071, 1.225733
C, -4.752353, -0.223331, 0.967668
H, -2.933939, -0.505387, 2.102743
H, -3.590872, -1.993633, 1.409333
H, -5.241526, -0.64917, 0.089741
H, -4.581237, 0.84084, 0.791878
H, -5.419509, -0.327031, 1.826988
H, -1.245441, -1.959033, 0.034614
O, -0.550883, -2.646658, -0.093962
C, -0.910431, -3.434519, -1.22751
C, -2.18156, -4.226936, -0.969206
H, -0.068365, -4.102876, -1.412909
H, -1.031189, -2.790112, -2.103505
H, -3.018212, -3.548159, -0.790662
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H, -2.42586, -4.854952, -1.829554
H, 1.075011, -2.058197, -0.035832
O, 2.018155, -1.801457, 0.092168
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C, 2.56872, -4.003664, 0.968765
H, 1.902065, -2.28749, 2.102175
H, 3.520434, -2.112491, 1.411205
H, 3.184076, -4.214731, 0.092297
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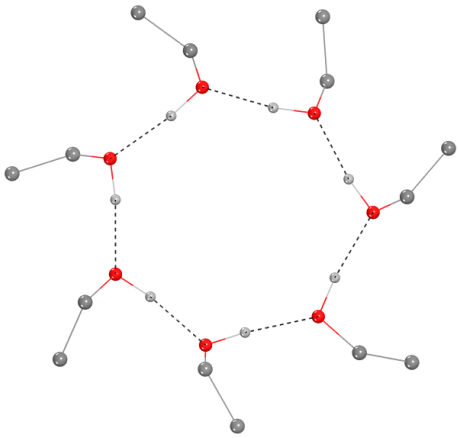
H, 2.990039, -4.529372, 1.8292

Cyclic-*gauche* $(EtOH)_7$



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C, 2.929436, -3.18327, 0.808227
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H, 2.347719, -1.445674, 0.080418
H, 3.85165, -3.869421, -1.015487
H, 4.625657, -2.446888, -0.306395
H, 4.877018, -4.045536, 0.42357
H, 2.425946, -4.129111, 1.014051
H, 3.219792, -2.745843, 1.76932
H, 0.268215, -2.727308, 0.105224
O, -0.646869, -3.025361, -0.094642
C, -0.653299, -3.584085, -1.407591
C, 0.102106, -4.902089, -1.453514
H, -0.222471, -2.869811, -2.115187
H, -1.702318, -3.731026, -1.66954
H, -0.325574, -5.606437, -0.737647

H, 1.152928, -4.742761, -1.202941
H, 0.050411, -5.341097, -2.453001
H, -1.936123, -1.909186, 0.193492
O, -2.748732, -1.390501, 0.396378
C, -3.451036, -2.045707, 1.449478
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H, -4.245222, -1.363719, 1.757313
H, -2.783219, -2.194392, 2.303136
H, -3.225289, -4.046431, 0.67994
H, -4.695425, -3.215907, 0.134857
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O, -2.888727, 1.292064, 0.051952
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H, -3.352859, 0.798384, -1.904611
H, -3.75215, 2.437789, -1.374273
H, -5.558036, 1.517845, 0.099595
H, -5.158713, -0.122664, -0.446747
H, -5.829034, 1.050895, -1.592185
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O, -0.755925, 2.960769, 0.069804
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C, -2.255886, 4.68212, 0.910761
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H, -1.192738, 3.205055, 2.078513
H, -3.140695, 4.058826, 0.765316
H, -2.097761, 5.280725, 0.011572
H, -2.442509, 5.354345, 1.752026
H, 0.896618, 2.493032, -0.162631
O, 1.849715, 2.371748, -0.378356
C, 2.14376, 3.115481, -1.558661
C, 2.033711, 4.611736, -1.313622
H, 1.473343, 2.808308, -2.366787
H, 3.16176, 2.843893, -1.842754
H, 2.702043, 4.91075, -0.503648
H, 1.009994, 4.873355, -1.037851
H, 2.301594, 5.17055, -2.213834
H, 2.658074, 0.844824, -0.168417
O, 3.228675, 0.07531, 0.058279
C, 4.017032, 0.44168, 1.188834
C, 4.974998, 1.573981, 0.85484
H, 4.57019, -0.453084, 1.479466
H, 3.364985, 0.723312, 2.021549
H, 4.414849, 2.467406, 0.57213
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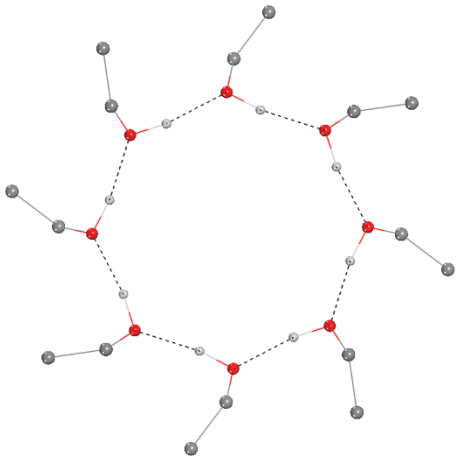
H, 5.600113, 1.816527, 1.717902

Cyclic-*gauche* $(EtOH)_8$



C, -5.538042, 0.990179, -0.976384
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H, -2.682691, -3.958049, 1.598348
H, -4.712205, -3.922877, 0.129534
H, -5.078423, -2.278017, 0.685676
H, -5.159672, -3.634087, 1.823519
H, -0.771987, -3.057838, 0.014467
O, 0.083394, -3.506179, -0.174394
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C, -0.990161, -5.538095, -0.976065
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H, -1.986457, -5.189779, -0.695885
H, -0.570559, -6.105471, -0.142915
H, -1.0868, -6.201525, -1.839223
H, 1.615116, -2.7084, -0.003778
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C, 3.016262, -3.151597, 1.308701
C, 3.227502, -4.61754, 0.966211
H, 2.315943, -3.048978, 2.142762
H, 3.958092, -2.682594, 1.59842
H, 3.922855, -4.712216, 0.129755
H, 2.278005, -5.07837, 0.685966
H, 3.634102, -5.159554, 1.823781

H, 3.057852, -0.771984, 0.014444
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H, 3.777469, -0.513728, -2.13756
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H, 6.201468, -1.086917, -1.839341
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C, 3.151651, 3.016309, 1.3085
C, 4.617575, 3.227559, 0.965935
H, 3.04908, 2.316014, 2.142588
H, 2.682648, 3.958142, 1.598211
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H, -3.922859, 4.712222, 0.129362
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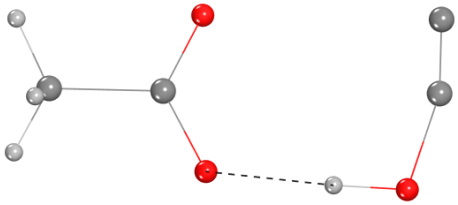
Gauche-$\left[\mathrm{OAc(EtOH)}\right]^-$



O, -0.97246, 1.057486, -0.582029
O, -0.93039, -1.027213, 0.280610
C, -1.50133, 0.047307, -0.071155
C, -3.02124, 0.082319, 0.181641
H, -3.45644, 1.014167, -0.180172
H, -3.49042, -0.770276, -0.315333
H, -3.20755, -0.023053, 1.253633
C, 2.184226, 0.01289, -0.497571
H, 1.525691, 0.407987, -1.277212
H, 3.191198, -0.107108, -0.913318
C, 2.210626, 1.000879, 0.664122
H, 2.597147, 1.974776, 0.342379
H, 1.192753, 1.140551, 1.030894
H, 2.839299, 0.615468, 1.472135
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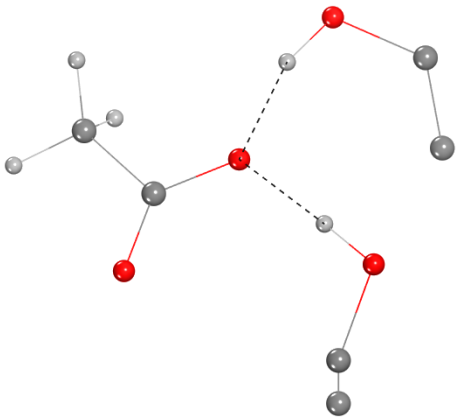
H, 0.770253, -1.211203, 0.050098

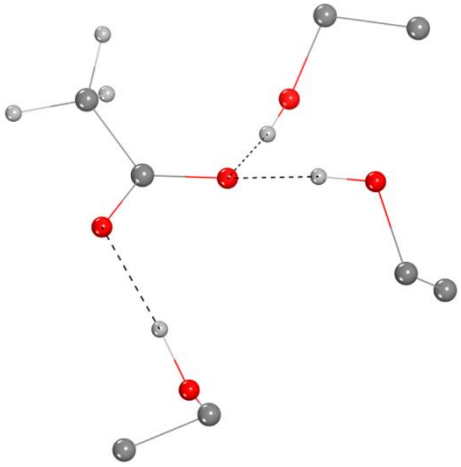
Gauche-$\left[\mathrm{OAc(EtOH)_2}\right]^-$



O, -0.16671, 0.803228, -0.449171
O, 1.733615, 1.877949, 0.083347
C, 0.499797, 1.81185, -0.033266
C, -0.35132, 3.029432, 0.347433
H, -0.90646, 3.36827, -0.530723
H, -1.08625, 2.738706, 1.102073
H, 0.275549, 3.836512, 0.725022
O, 1.194644, -1.475124, -1.121979
C, 2.431567, -1.376365, -0.44499
H, 3.048102, -2.210924, -0.794184
H, 2.933053, -0.437977, -0.701006
C, 2.257934, -1.44765, 1.068325
H, 3.22856, -1.42407, 1.575853
H, 1.675331, -0.587751, 1.403118
H, 1.732124, -2.365763, 1.344736
H, 0.701371, -0.637376, -0.939609
O, -2.79458, 0.193571, -0.316514
C, -2.57493, -1.203897, -0.34249
H, -3.54288, -1.673336, -0.542927
H, -1.89321, -1.468131, -1.158741
C, -2.0024, -1.71641, 0.974304
H, -1.03595, -1.244226, 1.157567
H, -2.67896, -1.471964, 1.797732

H, -1.85462, -2.800722, 0.941021
H, -1.89537, 0.599992, -0.361286

Gauche-$\left[\mathrm{OAc}\left(\mathrm{EtOH}\right)_3\right]^-$



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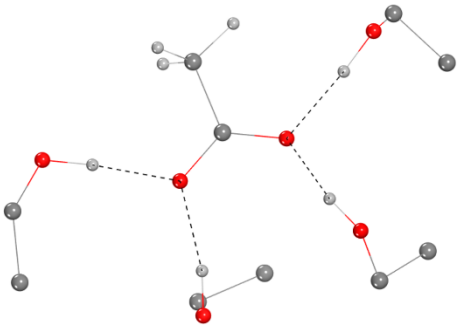
O, -1.495982, -1.666261, -1.168704
C, -0.340796, -1.658919, -0.695724
C, 0.427403, -2.979156, -0.646707
H, 1.163015, -2.976823, -1.456099
H, 0.97294, -3.065752, 0.294294
H, -0.248789, -3.82188, -0.784045
O, 0.647684, 1.803245, -1.514662
C, -0.210399, 2.636735, -0.754249
H, -0.238971, 3.603673, -1.264525
H, -1.224813, 2.227064, -0.746276
C, 0.30099, 2.81346, 0.6722
H, -0.373226, 3.450632, 1.254591
H, 0.373492, 1.840963, 1.164086
H, 1.296567, 3.264887, 0.664799
O, 2.394328, -0.944194, 1.428835
C, 3.476574, -0.779156, 0.536327
H, 4.358091, -1.20094, 1.027952
H, 3.302075, -1.35288, -0.383493
C, 3.718519, 0.68518, 0.187901
H, 2.852016, 1.105473, -0.326382
H, 3.889186, 1.258293, 1.102933
H, 4.593421, 0.791384, -0.462826
H, 1.57067, -0.806213, 0.902837
H, 0.50016, 0.888865, -1.191337
O, -3.087108, 0.500657, -0.544968
C, -2.813971, 0.488446, 0.843017
H, -1.737819, 0.381545, 1.012413
H, -3.127065, 1.459629, 1.238944
C, -3.563901, -0.633339, 1.554977
H, -3.247944, -1.596968, 1.150215
H, -3.36208, -0.620386, 2.631272
H, -4.639786, -0.527048, 1.394281
H, -2.533628, -0.214072, -0.935268

Gauche-$\left[\mathrm{OAc}\left(\mathrm{EtOH}\right)_4\right]^-$



O, 0.981734, -0.563675, 0.081442
O, -1.231533, -0.614423, -0.230790
C, -0.144075, -1.128092, 0.150548
C, -0.217468, -2.531321, 0.740502
H, -0.640882, -3.207303, -0.005305
H, 0.76509, -2.881472, 1.053153
H, -0.901334, -2.527727, 1.591983
O, 1.8835, 1.290152, -1.79192
C, 1.735258, 2.505331, -1.077287
H, 1.977183, 3.308553, -1.778204
H, 0.695449, 2.636366, -0.761985
C, 2.665382, 2.564813, 0.129881
H, 2.547105, 3.510082, 0.670056
H, 2.442215, 1.74317, 0.813963
H, 3.705965, 2.468463, -0.190077
O, 3.227696, -1.689049, 1.202898
C, 3.895133, -2.118415, 0.032301
H, 4.630285, -2.863869, 0.347473
H, 3.189253, -2.612115, -0.647925
C, 4.586555, -0.968681, -0.690751
H, 3.855452, -0.232962, -1.03164
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H, 5.140182, -1.33422, -1.562166
H, 2.416759, -1.217557, 0.909116
H, 1.486697, 0.588989, -1.234917
O, -1.85682, 2.061418, -0.202851
C, -2.051325, 2.06402, 1.19907
H, -2.692141, 2.920609, 1.424897
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H, -0.221562, 3.103836, 1.685176
H, -0.897509, 2.166487, 3.036887

H, -0.07826, 1.341479, 1.691555
H, -1.501126, 1.174106, -0.425049
O, -3.613346, -1.937153, 0.097091
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H, -5.257038, -2.089496, -1.065638
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H, -3.993992, 0.676409, -0.64515
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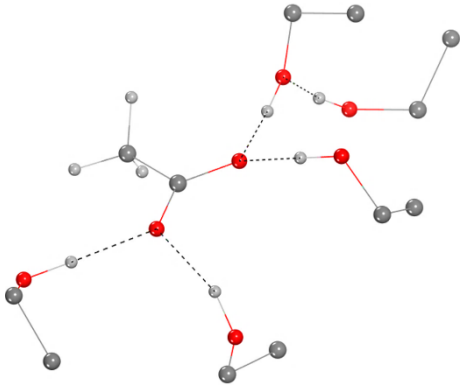
H, -5.408805, 0.051651, 0.223789

Gauche-$\left[\mathrm{OAc}\left(\mathrm{EtOH}\right)_5\right]^-$



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H, 0.351468, -2.8226, -1.418426
H, 0.829362, -2.90754, 0.284754
H, -0.886537, -2.64541, -0.173208
O, 3.080216, 1.4883, -1.382507
C, 2.967192, 2.555263, -0.455034
H, 3.474542, 3.411368, -0.906915
H, 1.915806, 2.823066, -0.312018
C, 3.612516, 2.207909, 0.882084
H, 3.529995, 3.042819, 1.585886
H, 3.121524, 1.335703, 1.319193
H, 4.669337, 1.968541, 0.740473
O, 3.366147, -2.18757, 1.061871
C, 4.170904, -2.52642, -0.051072
H, 4.709021, -3.43868, 0.219375
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C, 5.154798, -1.41868, -0.40778
H, 4.62347, -0.51028, -0.698705
H, 5.782495, -1.19064, 0.457285
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H, 2.708938, -1.53135, 0.744244
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H, 0.633111, 2.838108, 1.98243
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C, -2.708026, -0.99832, 2.24751
H, -2.670832, -2.02874, 2.607908
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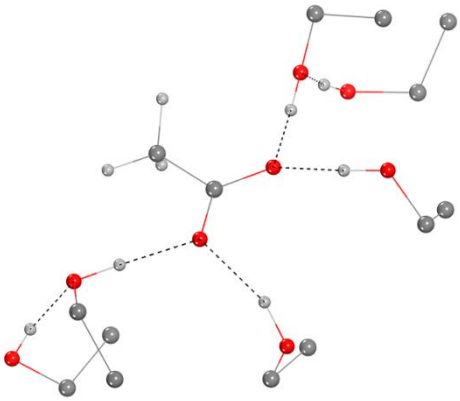
H, -2.37423, -0.33146, 3.04834

Gauche-$\left[\mathrm{OAc}\left(\mathrm{EtOH}\right)_6\right]^-$



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C, -0.49683, -1.646353, -1.609002
H, 0.219687, -1.767473, -2.422699
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H, -1.49818, -1.918237, -1.940153
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C, 1.625528, 3.247786, 0.485321
H, 1.941292, 4.292114, 0.546172
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C, 2.602175, 2.359077, 1.248707
H, 2.628907, 2.627437, 2.309876
H, 2.301106, 1.312414, 1.164561
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O, 2.925442, -1.212133, -0.962068
C, 3.580551, -0.761104, -2.137352
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H, -4.19339, 1.716199, -0.058324
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O, -5.02777, -2.440129, 0.261093
H, -4.66898, -1.84055, -0.425266
C, -4.40143, -2.113734, 1.487388
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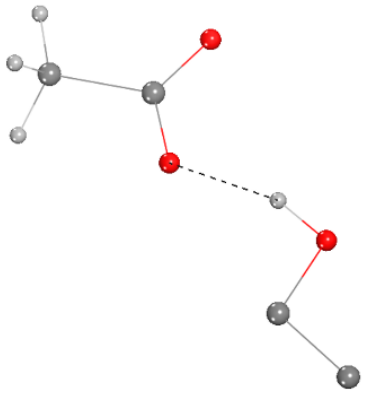
H, -2.6847, -3.381568, 1.172403
H, -2.42227, -1.686106, 0.723666
H, -2.44672, -2.146465, 2.429749
O, 4.26862, -2.42835, 1.140368
H, 3.724871, -2.139842, 0.381427
C, 5.0867, -1.333619, 1.504905
H, 4.556117, -0.390444, 1.335365
H, 5.281959, -1.418759, 2.576973
C, 6.405086, -1.339918, 0.738718
H, 6.218813, -1.262922, -0.334956
H, 7.041848, -0.502579, 1.041104
H, 6.937915, -2.27503, 0.924401

Trans-$\left[\mathrm{OAc}\left(\mathrm{EtOH}\right)\right]^{-}$



O, -2.331578, 1.318065, -0.027571
O, -0.809361, -0.349408, 0.030768
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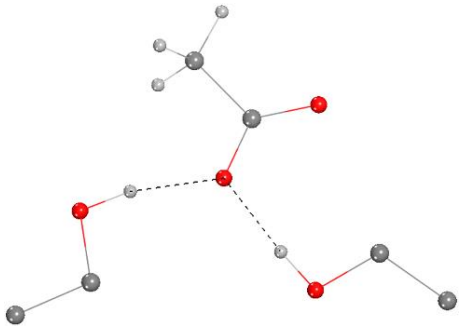
C, -3.099502, -0.94846, -0.003164
H, -4.086409, -0.486219, -0.038345
H, -2.963858, -1.607269, -0.864743
H, -3.007858, -1.564556, 0.895113
C, 2.250327, -0.436449, -0.019605
H, 1.966558, -0.987979, -0.925801
H, 1.97128, -1.064657, 0.83665
C, 3.751618, -0.190185, -0.013536
H, 4.308765, -1.131445, -0.057932
H, 4.030226, 0.42612, -0.871663
H, 4.036443, 0.346729, 0.894431
O, 1.595288, 0.805232, 0.036272
H, 0.61978, 0.600571, 0.037298

Trans-$\left[\mathrm{OAc(EtOH)_2}\right]^-$



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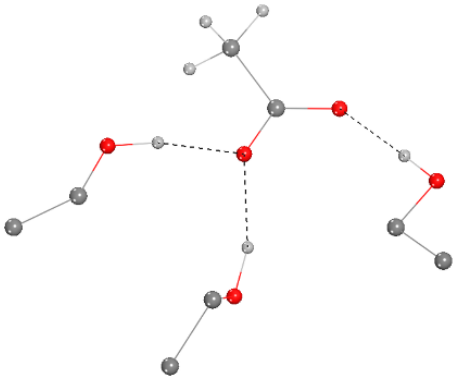
C, -0.492207, 3.09279, 0.016465
H, -1.155711, 3.056159, -0.850992
H, -1.12057, 3.005639, 0.906324
H, 0.049742, 4.037731, 0.033011
O, 1.462071, -1.484264, -0.233837
C, 2.639391, -1.138793, 0.468487
H, 2.780005, -0.054987, 0.446226
H, 2.55877, -1.449638, 1.521009
C, 3.824059, -1.846308, -0.173333
H, 4.749439, -1.641496, 0.374601
H, 3.654776, -2.926413, -0.185389
H, 3.941943, -1.508151, -1.204972
H, 0.874369, -0.689421, -0.219839
O, -2.704034, 0.18903, 0.040547
C, -2.579002, -1.215407, -0.027483
H, -2.073257, -1.514669, -0.953731
H, -1.971596, -1.590763, 0.804992
C, -3.970429, -1.824137, 0.025704
H, -4.468754, -1.534673, 0.953872
H, -4.570289, -1.456511, -0.810124
H, -3.924225, -2.915804, -0.025357
H, -1.779754, 0.545664, 0.009644

Trans-$\left[\mathrm{OAc(EtOH)_3}\right]^-$



O, 0.02658, 1.058072, 0.059403
O, 1.790831, 2.301438, -0.564457
C, 0.612485, 2.162589, -0.182515
C, -0.237366, 3.417543, 0.02259
H, -1.105765, 3.375631, -0.639464
H, -0.615442, 3.438159, 1.047033
H, 0.344811, 4.314653, -0.181927
O, -0.281816, -1.374764, -1.130613
C, -0.568424, -2.09631, 0.051212
H, 0.360849, -2.435247, 0.529845
H, -1.097911, -1.460167, 0.768551
C, -1.422707, -3.297309, -0.318974
H, -1.649478, -3.903715, 0.562518
H, -2.360905, -2.962777, -0.767877
H, -0.897806, -3.917923, -1.048975
O, -2.496505, 0.844449, 1.012862
C, -3.181539, 0.442764, -0.157227
H, -3.523182, 1.321504, -0.723258
H, -2.517622, -0.133849, -0.809119
C, -4.381653, -0.398223, 0.247488
H, -4.045858, -1.291711, 0.778798
H, -5.029917, 0.172417, 0.916914
H, -4.960676, -0.704516, -0.628674
H, -1.554597, 1.00471, 0.758901
H, 0.001656, -0.474549, -0.855714
O, 3.714235, 0.350193, -0.103288
C, 2.968707, -0.806944, 0.222974
H, 2.229347, -0.580597, 0.999428
H, 2.417257, -1.174677, -0.649673
C, 3.93692, -1.871066, 0.711256
H, 4.474899, -1.51347, 1.592433
H, 3.405997, -2.792083, 0.969347
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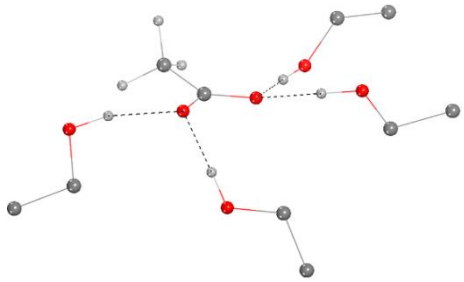
H, 3.069319, 1.059481, -0.323518

Trans-$\left[\mathrm{OAc(EtOH)_4}\right]^-$



O, -0.551992, -0.709413, 0.027397
O, 1.584526, -0.649741, 0.68994
C, 0.575837, -1.241358, 0.223522
C, 0.725008, -2.725001, -0.097019
H, 0.617867, -3.285599, 0.835571
H, -0.046279, -3.055802, -0.791878
H, 1.719531, -2.927491, -0.49577
O, -2.224028, 1.145955, 1.180779
C, -2.850448, 1.586245, -0.009277
H, -2.286134, 2.416325, -0.455848
H, -2.887998, 0.775729, -0.744724
C, -4.255574, 2.04953, 0.336453
H, -4.772383, 2.426791, -0.550399
H, -4.830234, 1.219025, 0.752794
H, -4.212837, 2.844074, 1.084923
O, 4.160011, -1.56521, 0.482314
H, 3.212197, -1.369159, 0.652247
C, 4.718604, -0.388676, -0.073835
H, 4.189071, -0.106869, -0.991063
H, 4.622783, 0.45148, 0.623198
C, 6.182878, -0.656385, -0.374057
H, 6.274524, -1.486725, -1.07791
H, 6.66044, 0.22742, -0.805598
H, 6.708381, -0.929011, 0.543917
O, -2.763778, -1.882146, -1.05674
C, -3.600311, -1.958277, 0.083109
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H, -3.389773, -1.129544, 0.766399
C, -5.047684, -1.906792, -0.377312
H, -5.240411, -0.962241, -0.891035
H, -5.247253, -2.721982, -1.076803
H, -5.73264, -1.993928, 0.470985
H, -1.898696, -1.517362, -0.761218
H, -1.472786, 0.571427, 0.92239
O, 2.006624, 2.046847, 0.118967
C, 0.731812, 2.565148, -0.215613
H, 0.24565, 1.929644, -0.964459
H, 0.079079, 2.587919, 0.664134
C, 0.921981, 3.969703, -0.760734
H, 1.559955, 3.945186, -1.647109
H, -0.039744, 4.4165, -1.02851
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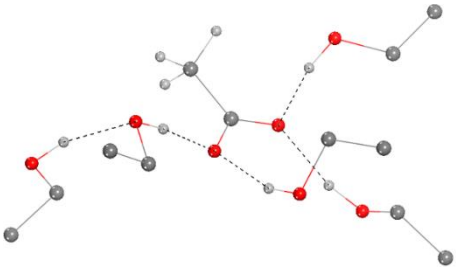
H, 1.87842, 1.114366, 0.394402

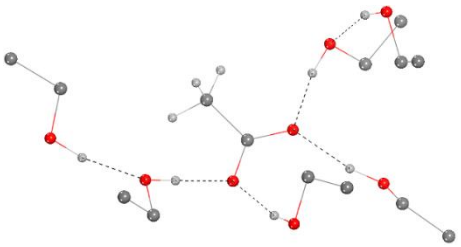
Trans-$\left[\mathrm{OAc(EtOH)_5}\right]^-$



O, -0.859244, -0.196475, 0.077606
O, 1.165004, -1.145316, 0.12398
C, -0.037134, -1.102472, -0.241781
C, -0.545023, -2.244076, -1.114531
H, -0.796714, -3.084148, -0.461846
H, -1.43812, -1.953253, -1.667461
H, 0.238006, -2.574133, -1.797815
O, 0.113501, 2.366841, 0.318983
C, 0.847978, 2.308403, -0.890318
H, 1.517826, 1.441584, -0.886169
H, 0.168661, 2.197464, -1.746383
C, 1.646614, 3.592784, -1.023685
H, 2.214772, 3.603984, -1.957686
H, 0.975185, 4.45433, -1.008431
H, 2.34254, 3.688011, -0.187027
O, -4.98909, -1.167704, 0.089888
H, -4.423277, -0.667311, -0.533417
C, -4.139355, -1.639997, 1.123192
H, -3.464972, -2.416216, 0.741144
H, -3.512992, -0.827763, 1.507306
C, -5.009495, -2.207341, 2.22949
H, -5.632194, -3.014681, 1.837951
H, -4.395534, -2.598255, 3.04462
H, -5.6668, -1.429476, 2.623499
O, -3.112917, 0.393781, -1.225815
C, -3.374288, 1.699924, -0.72319
H, -3.561921, 1.654638, 0.356226
H, -2.501744, 2.340081, -0.880916
C, -4.591584, 2.250486, -1.442457
H, -4.404599, 2.290345, -2.517551
H, -5.455614, 1.606343, -1.264626
H, -4.826644, 3.256962, -1.087042
H, -2.273847, 0.082348, -0.797494
H, -0.251119, 1.467556, 0.461853
O, 2.844112, -0.161979, 2.129935

C, 3.119363, 1.159467, 1.702619
H, 3.609099, 1.150219, 0.7182
H, 2.194317, 1.73542, 1.607996
C, 4.041205, 1.802453, 2.723764
H, 4.963278, 1.223651, 2.815066
H, 4.293336, 2.825421, 2.430728
H, 3.55425, 1.825886, 3.70078
H, 2.167841, -0.531504, 1.527452
O, 3.173651, -2.495309, -1.17858
H, 2.380853, -2.154035, -0.7117
C, 4.191814, -1.527103, -1.005786
H, 3.9082, -0.582711, -1.489314
H, 4.346504, -1.319581, 0.058496
C, 5.467234, -2.06419, -1.630772
H, 5.306419, -2.270223, -2.691328
H, 6.284514, -1.344802, -1.530345
H, 5.756385, -2.996889, -1.142026

Trans-$\left[\mathrm{OAc}\left(\mathrm{EtOH}\right)_6\right]^-$



O, 1.007633, 0.412457, -1.35905
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C, 0.392549, -0.628451, -0.995071
C, 1.238188, -1.848517, -0.656443
H, 2.023721, -1.978275, -1.402323
H, 1.725719, -1.669769, 0.305517
H, 0.626932, -2.747033, -0.584946
O, 0.126616, 2.844015, -0.419147
C, -0.173275, 2.379262, 0.88513
H, -0.852754, 1.521654, 0.837435
H, 0.742138, 2.045754, 1.393238
C, -0.813939, 3.515705, 1.660714
H, -1.042738, 3.207948, 2.684179
H, -0.140459, 4.375224, 1.690652
H, -1.740397, 3.824626, 1.170994
O, 5.708127, -1.113369, -0.697087
H, 4.977801, -0.482012, -0.857615
C, 5.462486, -1.723818, 0.554913
H, 5.35795, -0.963722, 1.338639
H, 4.528573, -2.298387, 0.527599
C, 6.628065, -2.64374, 0.870332
H, 7.556112, -2.069726, 0.91061
H, 6.480603, -3.146205, 1.829778
H, 6.72798, -3.399255, 0.088514
O, 3.576809, 0.643153, -0.670224
C, 3.758963, 2.037507, -0.461569
H, 4.106051, 2.510004, -1.38783
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C, 4.786654, 2.231899, 0.639876
H, 4.421274, 1.796604, 1.572443
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H, 4.985752, 3.294604, 0.801331
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H, 0.378485, 2.055561, -0.944685
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H, -3.353198, 1.835815, -0.029562
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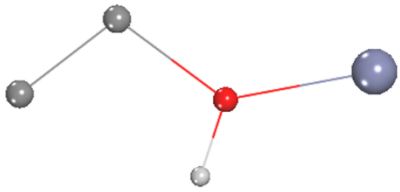
C, -4.349666, 2.716092, -1.719428
H, -5.275495, 2.150858, -1.589948
H, -4.464865, 3.694985, -1.246171
H, -4.182034, 2.858287, -2.788895
H, -2.256095, 0.271243, -1.500862
O, -2.315286, -2.850506, -0.08439
H, -1.684683, -2.135061, -0.341828
C, -3.413379, -2.794194, -0.992142
H, -3.750313, -1.760523, -1.109453
H, -3.09594, -3.158126, -1.975835
C, -4.52861, -3.66615, -0.444201
H, -4.859634, -3.290512, 0.526456
H, -5.381619, -3.672429, -1.127571
H, -4.174766, -4.69133, -0.313529
O, -3.189765, -1.743094, 2.3362
H, -2.864918, -2.309481, 1.609012
C, -3.328783, -0.435057, 1.80014
H, -2.500429, -0.214731, 1.120822
H, -4.258079, -0.354686, 1.220229
C, -3.345826, 0.555828, 2.949907
H, -2.404379, 0.502898, 3.500879
H, -3.480909, 1.576188, 2.581303
H, -4.160236, 0.318725, 3.638447

Gauche-$\left[\mathrm{Zn(EtOH)}\right]^{2+}$



Zn, 1.443589, 0.012616, 0.013369
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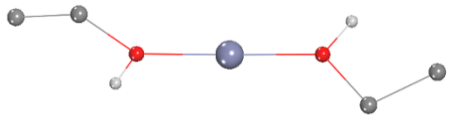
C, -1.672298, 0.648143, -0.03387
H, -1.487787, 1.249974, 0.849285
H, -1.564234, 1.189919, -0.967098
C, -2.851657, -0.256668, 0.04934
H, -2.881234, -0.833392, 0.974497
H, -3.728137, 0.408069, 0.064553
H, -2.965088, -0.890732, -0.831874

Gauche-$\left[\mathrm{Zn(EtOH)_2}\right]^{2+}$



Zn, -0.002484, -0.249111, -0.04862
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O, 1.817689, -0.18466, -0.335897
H, 2.201837, -0.500494, -1.176428
H, -2.247491, -1.065198, 0.653914
C, 2.980436, 0.199081, 0.634172
H, 2.627704, 1.113104, 1.101391
H, 3.02823, -0.631044, 1.331583
C, 4.218126, 0.379949, -0.191786
H, 4.115306, 1.190156, -0.914198
H, 5.028127, 0.651189, 0.492137
H, 4.521176, -0.546334, -0.684814
C, -2.921533, 0.771278, -0.086746
H, -2.768151, 1.527982, 0.675857
H, -2.66154, 1.124981, -1.079489
C, -4.254541, 0.089334, -0.017219
H, -4.467144, -0.294613, 0.982918
H, -5.017009, 0.844118, -0.232662
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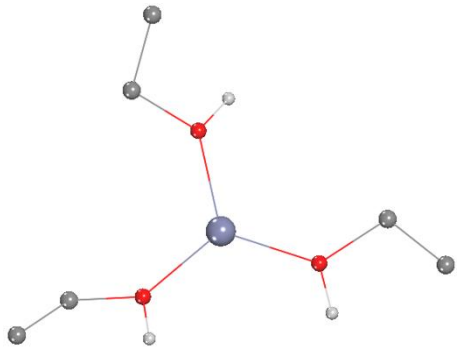
Gauche-$\left[\mathrm{Zn(EtOH)_3}\right]^{2+}$



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O, -1.264964, -1.451133, 0.19674
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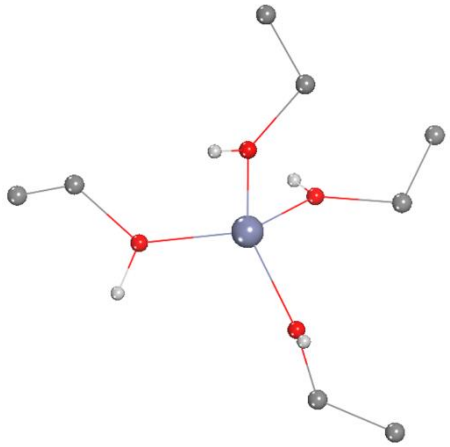
H, 2.97926, 0.823532, 0.545199
H, 3.503201, 0.319143, -1.093035
C, 4.344537, -0.864432, 0.528872
H, 4.59638, -1.716335, -0.107145
H, 5.248884, -0.258879, 0.621095
H, 4.066879, -1.209604, 1.52475
C, -2.632252, -1.51764, -0.449145
H, -2.875357, -0.479753, -0.661686
H, -2.498797, -2.077891, -1.370556
C, -3.5974, -2.163544, 0.507655
H, -3.685765, -1.599331, 1.436255
H, -4.581517, -2.19406, 0.034828
H, -3.317698, -3.197215, 0.724267
C, -1.472649, 2.364834, 0.041615
H, -2.161857, 2.329052, -0.79819
H, -1.846788, 1.777135, 0.876303
C, -1.089304, 3.765185, 0.437277
H, -0.687863, 4.326835, -0.409408
H, -1.989952, 4.287805, 0.767064
H, -0.375171, 3.770134, 1.260546

Gauche-$\left[\mathrm{Zn(EtOH)_5}\right]^{2+}$



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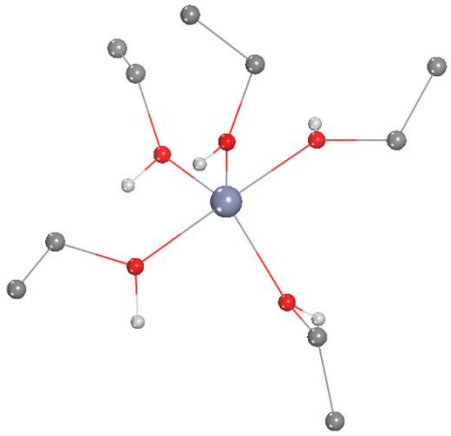
O, -0.634159, 0.518814, 1.422594
O, -1.496775, -0.976611, -1.182891
H, -1.624774, -0.849768, -2.136416
O, 1.029043, 1.102423, -1.251217
H, -0.264383, 0.328084, 2.299385
H, 1.549465, 0.920562, -2.049716
H, 1.18429, -2.624673, 0.304048
C, 2.894236, -1.52934, 0.327384
H, 3.047789, -0.491598, 0.61297
H, 3.267026, -1.700165, -0.6803
C, -2.558503, -1.874825, -0.651551
H, -2.301377, -2.885317, -0.961669
H, -2.46875, -1.785909, 0.429064
C, 0.901902, 2.576283, -1.066011
H, 0.064085, 2.898005, -1.68091
H, 0.663653, 2.693966, -0.011668
C, -1.904375, 1.27887, 1.56214
H, -2.683943, 0.55471, 1.790644
H, -2.074892, 1.705357, 0.575888
C, -1.761508, 2.331995, 2.632357
H, -2.696934, 2.889049, 2.709357
H, -1.572438, 1.883921, 3.610554
H, -0.963872, 3.037009, 2.396404
C, 2.195513, 3.252527, -1.443847
H, 2.431973, 3.101991, -2.499877
H, 2.090599, 4.328035, -1.289886
H, 3.023985, 2.900572, -0.828719
C, -3.908823, -1.434389, -1.157777
H, -3.971816, -1.511232, -2.245554
H, -4.674422, -2.093703, -0.744601
H, -4.135979, -0.412088, -0.853729
C, 3.467708, -2.497379, 1.33087
H, 4.550265, -2.363324, 1.370936
H, 3.066037, -2.323144, 2.329117
H, 3.28359, -3.533503, 1.037303

Gauche-$\left[\mathrm{Zn(EtOH)_5}\right]^{2+}$



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O, 1.396929, -1.391525, -0.552082
O, 0.929815, 1.190525, -1.515671
O, -1.767829, 1.238942, -0.205944
H, -0.614069, 0.502844, 2.159185
H, 1.997945, -1.301746, -1.307569
C, -2.492077, -2.108823, 0.114788
C, 1.292342, -0.082072, 2.498878
C, 1.473376, -2.753046, -0.004301
C, 2.116642, 1.928369, -1.038801
C, -1.717025, 2.691048, 0.015324
H, 0.930143, -3.416402, -0.676946
H, 2.620346, 1.230055, -0.372808
H, -0.854943, 2.839058, 0.663771
H, 2.069155, -0.411031, 1.813667
H, 0.946988, -2.694124, 0.946684
H, -1.530861, 3.170745, -0.945324
C, 2.913356, -3.177109, 0.166718
H, 2.947353, -4.180798, 0.593356
H, 3.432582, -3.215305, -0.793673
H, 3.448772, -2.502832, 0.836138
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H, -1.448854, -2.057246, -1.609379
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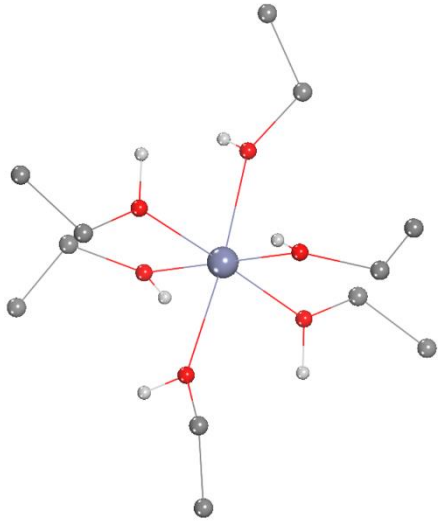
Gauche-$\left[\mathrm{Zn(EtOH)_6}\right]^{2+}$



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H, 2.210544, 2.890685, -1.172607
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H, -1.264665, -2.716577, 2.272984
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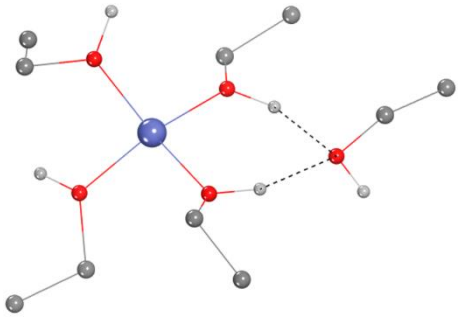
Gauche-$\left[\mathrm{Zn(EtOH)_4}\right]^{2+}(\mathrm{EtOH})$



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H, 3.243036, -1.710929, 2.261548
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H, 2.311548, -0.568228, 4.302477
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H, -5.69351, 0.974203, 1.075892
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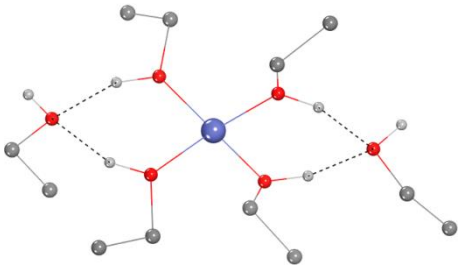
H, -3.089904, 1.116278, -1.37797

$\left[\mathrm{Zn(EtOH)_4}\right]^{2+}(\mathrm{EtOH})_2$



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O, 1.007212, -1.188488, -0.631928
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H, -2.418014, 0.878415, -0.759599
C, -1.503491, 1.714565, -2.395305
H, -0.525925, 1.535764, -2.836992
H, -1.584752, 2.762625, -2.11192
C, 1.543193, 2.776727, 1.141089
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H, -0.386426, -2.641294, -0.975009
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H, -3.226932, -1.517516, -1.199193
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H, 3.97129, 0.21792, -1.318474
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H, 4.715762, -2.462283, -0.455774
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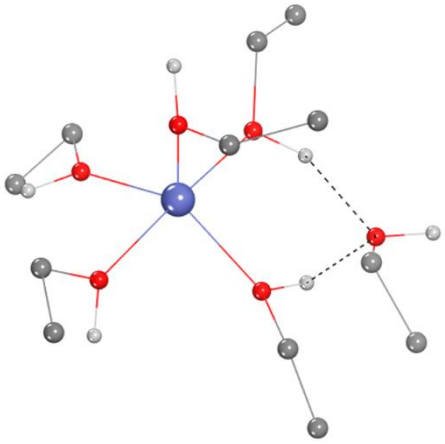
$\left[\mathrm{Zn(EtOH)_5}\right]^{2+}\left(\mathrm{EtOH}\right)$



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C, -0.54434, -2.756932, -0.407858
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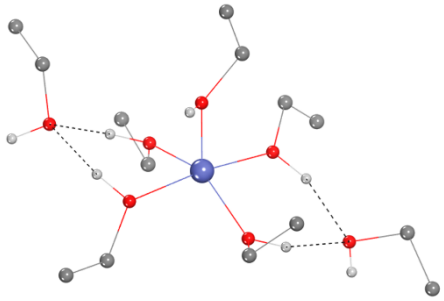
$\left[Zn(EtOH)_5\right]^{2+}(EtOH)_2$



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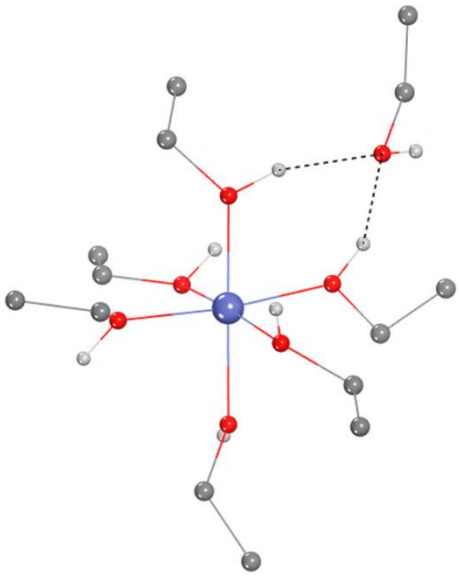
$\left[Zn(EtOH)_6\right]^{2+}(EtOH)$



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C, 2.011695, 1.7663, -2.150988
H, 1.069263, 1.585015, -2.664293
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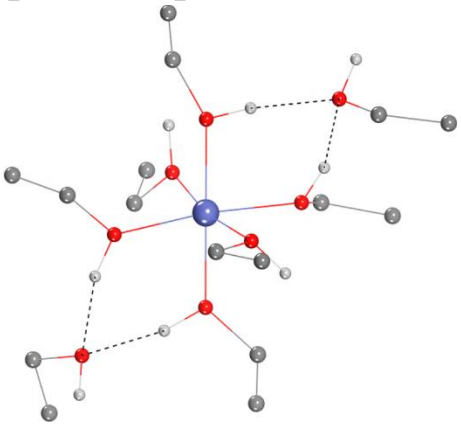
$\left[\mathrm{Zn(EtOH)_6}\right]^{2+}\mathrm{(EtOH)_2}$



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H, 0.26310443, 2.86468301, 1.78352494
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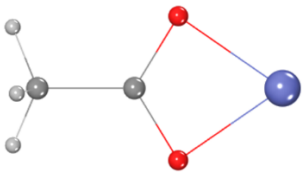
$[Zn(OAc)]^+$



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O, 0.385158, -1.095572, -0.008578
C, 2.543451, 0.000508, 0.002649
H, 2.858331, -0.080373, 1.047162
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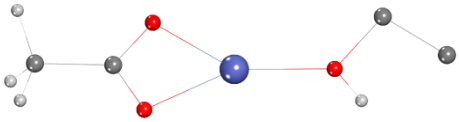
H, 2.921034, 0.931992, -0.41019

$[Zn(OAc)(EtOH)]^+$



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C, -2.31121, 0.15771, 0.046121
O, -1.846692, -1.037456, 0.085173
C, -3.770088, 0.427883, 0.143885
H, -4.332781, -0.406911, -0.266661
H, -4.020526, 0.525996, 1.203638
O, 1.829364, -0.504047, -0.140929
H, 2.244486, -1.382044, -0.134625
C, 2.854879, 0.56246, -0.375601
H, 3.06977, 0.547081, -1.440977
H, 2.346207, 1.485167, -0.108563
C, 4.062639, 0.29349, 0.483321
H, 4.793799, 1.085944, 0.312718
H, 3.804341, 0.287957, 1.542098
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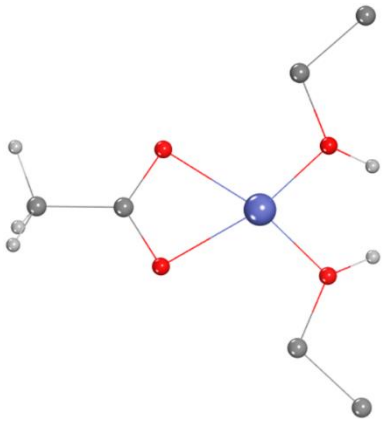
$\left[Zn(OAc)(EtOH)_2\right]^+$



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O, -1.546939, -1.281465, -0.372188
O, 1.553559, -1.276571, 0.359594
C, 0.000038, 2.233611, 0.009977
C, -0.022037, 3.725632, 0.001625
H, 0.900198, 4.110894, -0.42708
H, -0.852622, 4.047728, -0.631371
H, -0.18372, 4.105679, 1.007111
C, 2.934913, -0.759768, 0.229073
C, 3.862874, -1.874593, -0.187279
H, 3.552968, -2.306521, -1.138778
H, 4.871275, -1.473768, -0.303171
H, 3.908152, -2.661443, 0.56923
H, 2.855755, 0.021616, -0.522291
H, 3.205596, -0.319177, 1.18685
H, 1.532368, -2.037666, 0.958334
C, -2.931266, -0.776913, -0.227107
C, -3.845033, -1.899541, 0.199587
H, -4.855669, -1.507506, 0.325643
H, -3.89112, -2.68737, -0.555835
H, -3.521512, -2.327943, 1.148144
H, -2.851023, 0.005541, 0.523093
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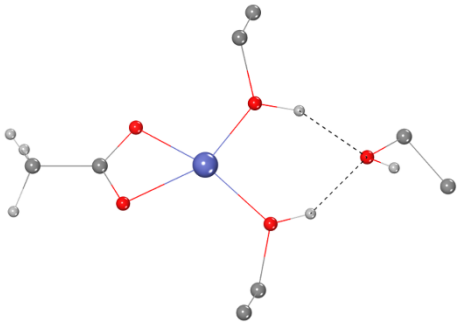
H, -1.524292, -2.040116, -0.973955

$\left[Zn(OAc)(EtOH)_2\right]^+(EtOH)$



Zn, 0.690042, -0.024966, 0.106068
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O, -0.389118, 1.31245, 1.078098
O, -0.730387, -1.30962, -0.386283
C, 2.984146, -0.048372, -0.384407
C, 4.4491, -0.047815, -0.672821
H, 4.632331, 0.305248, -1.684738
H, 4.930592, 0.640531, 0.026087
H, 4.863067, -1.04086, -0.51593
C, -0.461353, -2.75176, -0.378638
C, -0.152078, -3.238286, 1.019112
H, -0.991278, -3.061429, 1.695277
H, 0.03888, -4.312834, 0.997062
H, 0.741541, -2.748682, 1.411854
H, -1.334847, -3.236338, -0.811424
H, 0.382419, -2.880195, -1.051854
H, -1.600203, -1.088492, 0.009835
C, -0.058224, 2.738506, 0.999682
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H, -0.092, 4.34654, -0.413196
H, 0.243746, 2.771348, -1.135428
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H, -2.913404, 0.837178, -1.30778
C, -4.592087, -0.492958, -0.991334
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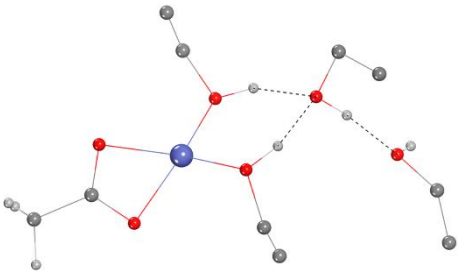
$\left[\mathrm{Zn(OAc)(EtOH)_2}\right]^{+}\left(\mathrm{EtOH}\right)_2$



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O, -0.66248, 1.242935, -1.115573
O, 0.072969, -0.457416, 1.254462
C, -3.61962, -1.058509, 0.003351
C, -4.99317, -1.642065, -0.058699
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C, 0.502752, -1.833348, 1.493759
C, 0.871962, -2.515941, 0.193451
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H, 1.230623, -3.527305, 0.39541
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H, 2.759099, 3.088785, 0.272816
H, 1.422295, 2.82943, 1.404324
C, 3.256981, 1.830881, 1.967046
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O, 3.687022, -0.093176, -1.153898
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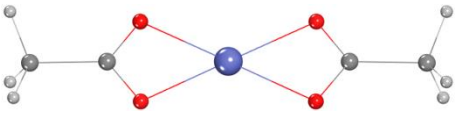
$\left[\mathrm{Zn(OAc)_2}\right]$



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O, 1.708417, 0.779694, -0.763516
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C, 3.849872, -0.019922, -0.004379
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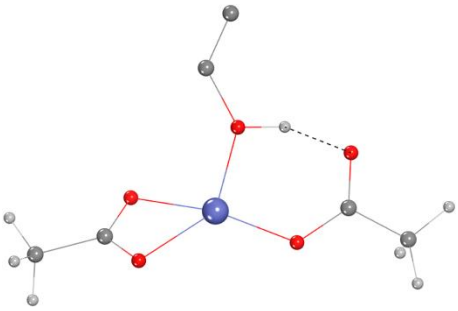
$\left[\mathrm{Zn(OAc)_2\ EtOH}\right]$



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C, 2.6179, -0.590861, 0.078701
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H, 0.978567, 2.598346, 0.270521

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H, -0.56442, 3.977333, -1.139868
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H, 4.471692, -0.14284, 1.043465
H, 4.326695, -1.788566, 0.400453
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H, -3.586, -2.705824, -0.591646
H, -3.39376, -2.612947, 1.154223
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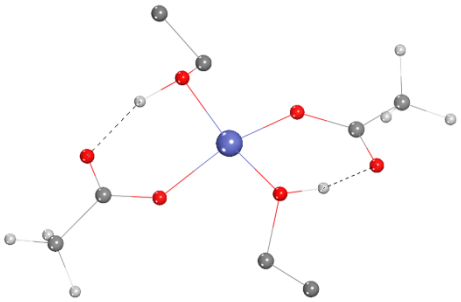
Tetrahedral-$\left[\mathrm{Zn(OAc)_2(EtOH)_2}\right]$



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O, 1.783598, 0.515282, -1.340252
O, -1.161125, -1.204674, -1.165593
C, 2.920839, 0.257796, -0.791002
C, -2.432508, -1.070614, -1.001177
C, -1.044025, 2.308673, 1.2075
H, -0.029566, 2.694782, 1.295219
H, -1.199166, 1.566471, 1.993097
C, -2.070172, 3.421861, 1.278575
H, -2.003454, 3.934067, 2.240842
H, -1.8984, 4.146333, 0.481729
H, -3.080106, 3.020428, 1.173128
H, -1.977036, 1.145967, -0.17721
C, -3.272552, -2.218616, -1.504913
H, -3.125183, -2.317236, -2.581543
H, -2.932928, -3.146351, -1.042684
H, -4.322554, -2.044997, -1.285003
O, 3.064413, -0.226561, 0.348148
C, 4.129491, 0.58838, -1.631004
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H, 4.074612, 0.033887, -2.568763
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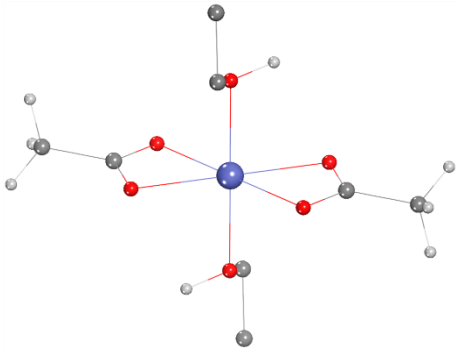
C, 0.331428, -1.83295, 1.794276
H, -0.757244, -1.835351, 1.832808
H, 0.650921, -2.575862, 1.059929
C, 0.93725, -2.103711, 3.157197
H, 0.630453, -3.088135, 3.517103
H, 2.027518, -2.082634, 3.103307
H, 0.609489, -1.350076, 3.874526

Octahedral-$\left[\mathrm{Zn(OAc)_2(EtOH)_2}\right]$



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O, -0.309648, -1.832897, 1.034305
O, -0.384596, 1.775444, 1.053036
C, 0.282526, -3.927707, 0.013778
C, -0.282525, 3.927707, -0.013779
H, 1.316135, -4.138697, 0.297815
H, -0.376347, -4.383898, 0.749544
H, 0.111392, -4.339802, -0.978925
H, -0.111391, 4.339802, 0.978924
H, 0.376347, 4.383898, -0.749546
H, -1.316135, 4.138697, -0.297816
O, 2.049775, 0.068317, 0.640322
O, -2.049775, -0.068317, -0.640322
H, 2.114888, 0.839137, 1.222697
H, -2.114889, -0.839137, -1.222696
C, 3.016589, 0.172438, -0.430758
H, 2.80976, 1.075787, -1.006029
H, 2.816518, -0.692609, -1.0591
C, -3.016588, -0.172438, 0.430759
H, -2.80976, -1.075787, 1.00603
H, -2.816517, 0.69261, 1.059101
C, 4.429183, 0.15248, 0.119334

H, 4.600043, -0.754907, 0.699869
H, 5.149671, 0.185563, -0.70067
H, 4.614065, 1.017377, 0.761913
C, -4.429183, -0.152479, -0.119332
H, -4.614066, -1.017376, -0.761911
H, -5.149671, -0.185562, 0.700673
H, -4.600043, 0.754908, -0.699867

Optimized geometries of Zinc complexes in solution phase at the M05-2X/6-31+G(d)/SMD level of theory.

Gauche-$(EtOH)_2$

C, -2.19606, 0.947441, -0.513066
C, -2.265769, -0.397512, 0.189226
O, -1.077412, -1.169545, -0.010879
H, -3.137944, 1.488742, -0.387562
H, -1.392662, 1.560711, -0.097391
H, -2.014417, 0.811118, -1.582009
H, -3.084596, -0.995437, -0.211535
H, -2.441303, -0.260056, 1.260739
H, -0.33342, -0.690587, 0.406541
C, 2.535818, -0.532592, -0.640626
C, 1.842248, 0.699545, -0.094154
O, 1.010708, 0.38588, 1.038093
H, 3.143047, -0.266542, -1.509613
H, 3.195008, -0.970786, 0.113574
H, 1.803834, -1.283989, -0.945673
H, 1.168435, 1.130073, -0.834539
H, 2.568674, 1.461996, 0.195759
H, 1.561548, -0.017215, 1.72571

Linear-*gauche* $(EtOH)_3$

C, -1.645612, -2.255316, -0.23564
C, -2.324639, -1.121163, 0.505699
O, -2.639611, -0.024805, -0.373971
H, -3.194994, -0.353442, -1.096795
H, -2.319961, -2.687567, -0.979967
H, -0.746202, -1.900107, -0.743598
H, -1.360628, -3.043617, 0.465819
H, -3.239911, -1.463772, 0.993558
H, -1.667364, -0.6989, 1.265734
H, -0.998508, 0.644417, -0.808814
O, -0.05968, 0.919044, -0.873831
C, 0.03896, 2.303519, -0.505953
C, -0.452568, 2.552369, 0.908254
H, -0.523933, 2.907381, -1.222741
H, 1.093946, 2.561458, -0.599698
H, 0.115165, 1.95394, 1.624843
H, -1.51169, 2.299865, 1.001495
H, -0.330187, 3.607961, 1.165513
H, 0.889062, -0.062425, 0.335708
O, 1.421585, -0.592676, 0.965485
C, 2.388687, -1.332012, 0.214677
C, 3.383601, -0.421559, -0.483378
H, 1.881543, -1.972626, -0.514018
H, 2.898861, -1.9777, 0.930151
H, 3.897389, 0.211378, 0.244327
H, 2.876997, 0.221082, -1.208395
H, 4.13149, -1.014869, -1.016538

Linear-*gauche* $(EtOH)_4$

C, -0.275632, -1.883029, -2.080966
C, -0.629097, -2.483015, -0.734408
O, -2.015048, -2.269478, -0.403168
H, -2.565853, -2.656474, -1.100154
H, -0.87265, -2.344218, -2.872755
H, -0.460087, -0.806004, -2.087735
H, 0.77902, -2.057336, -2.305351
H, -0.420455, -3.555017, -0.717173
H, -0.065793, -2.00962, 0.070243
H, -2.182202, -0.491322, -0.18504
O, -2.106793, 0.476639, -0.040211
C, -2.589828, 0.78887, 1.275896
C, -1.830765, 0.033568, 2.351352
H, -3.659266, 0.568469, 1.327753
H, -2.457494, 1.864882, 1.392525
H, -0.76263, 0.258259, 2.297491
H, -1.968941, -1.044763, 2.239776
H, -2.194816, 0.323795, 3.34052
H, -0.402342, 0.982366, -0.1066
O, 0.517551, 1.331569, -0.118674
C, 0.626063, 2.282317, -1.187919
C, -0.286565, 3.474979, -0.970011
H, 0.398722, 1.790581, -2.138371
H, 1.671012, 2.592791, -1.20847
H, -0.051348, 3.970438, -0.025069
H, -1.333346, 3.161644, -0.949417
H, -0.16332, 4.197937, -1.780624
H, 1.75354, 0.041939, -0.415221
O, 2.53232, -0.540773, -0.541374
C, 3.412354, -0.322795, 0.564883
C, 2.826239, -0.847147, 1.863922
H, 3.638694, 0.744892, 0.651066
H, 4.339432, -0.844611, 0.325123
H, 2.621606, -1.917954, 1.786746
H, 1.892678, -0.330231, 2.101987

H, 3.524989, -0.6866, 2.689672

Linear-*gauche* $(EtOH)_5$

C, -2.380791, 2.099187, -1.384359
C, -2.557697, 0.693752, -1.923553
O, -3.541426, -0.047074, -1.176719
H, -4.386842, 0.424285, -1.220163
H, -3.312615, 2.664803, -1.471215
H, -2.081068, 2.07667, -0.334205
H, -1.61021, 2.623018, -1.95558
H, -2.849055, 0.711156, -2.976076
H, -1.635118, 0.121722, -1.83096
H, -2.912572, -0.344197, 0.489529
O, -2.468592, -0.531733, 1.344818
C, -2.079131, -1.914067, 1.364161
C, -1.170176, -2.261129, 0.198993
H, -2.974982, -2.540575, 1.357699
H, -1.56901, -2.064705, 2.31562
H, -0.312464, -1.585496, 0.171223
H, -1.707119, -2.184889, -0.749524
H, -0.802074, -3.285775, 0.301852
H, -1.054426, 0.535352, 1.531046
O, -0.289545, 1.142601, 1.651278
C, 0.420617, 0.774042, 2.843598
C, 1.340608, -0.41165, 2.613634
H, -0.300032, 0.558618, 3.63664
H, 0.9944, 1.652183, 3.140685
H, 2.059349, -0.191883, 1.820024
H, 0.768508, -1.299679, 2.335273
H, 1.896931, -0.637011, 3.527843
H, 0.614381, 0.999508, 0.12517
O, 1.061028, 1.015141, -0.751438
C, 1.611914, 2.326922, -0.937446
C, 2.734625, 2.612247, 0.043904
H, 0.816551, 3.070773, -0.83696
H, 1.978363, 2.357593, -1.963781
H, 3.540431, 1.882889, -0.067431
H, 2.366201, 2.572812, 1.072524
H, 3.14461, 3.610393, -0.132619
H, 2.40799, -0.210549, -0.860827
O, 3.148211, -0.849601, -0.933421
C, 2.606884, -2.171323, -0.862001
C, 1.737599, -2.494892, -2.064644
H, 2.03917, -2.288812, 0.066415
H, 3.461336, -2.847373, -0.817222
H, 2.322027, -2.429464, -2.985737
H, 0.899602, -1.796764, -2.13733
H, 1.333603, -3.507814, -1.981782

Linear-*gauche* $(EtOH)_6$

C, -3.673282, -1.471875, -1.360683
C, -3.711965, -1.6401, 0.145022
O, -4.431121, -0.569191, 0.78548
H, -5.33578, -0.550406, 0.438786
H, -4.683771, -1.50165, -1.777439
H, -3.209699, -0.521058, -1.633381
H, -3.095498, -2.282998, -1.811266
H, -4.171491, -2.591651, 0.421555
H, -2.708422, -1.606658, 0.56745
H, -3.56356, 1.000592, 0.585297
O, -3.01658, 1.81233, 0.505343
C, -2.354332, 2.042748, 1.759225
C, -1.535535, 0.840476, 2.193354
H, -3.098536, 2.29929, 2.517845
H, -1.717413, 2.913354, 1.601933
H, -0.8424, 0.544743, 1.403738
H, -2.185143, -0.006818, 2.425807
H, -0.955058, 1.081151, 3.0884
H, -1.825378, 1.603454, -0.795059
O, -1.182481, 1.492129, -1.531994
C, -0.287813, 2.615304, -1.549716
C, 0.849354, 2.451283, -0.557258
H, -0.855628, 3.527146, -1.347412
H, 0.101503, 2.679949, -2.566313
H, 1.415091, 1.542359, -0.77313
H, 0.473443, 2.393599, 0.467177
H, 1.531614, 3.303527, -0.624649
H, -0.483749, -0.096984, -1.170546
O, -0.188536, -1.008431, -0.944542
C, 0.234653, -1.663591, -2.147918
C, 1.575617, -1.142375, -2.632031
H, -0.53071, -1.530375, -2.91729
H, 0.294545, -2.726482, -1.912681
H, 2.344966, -1.290399, -1.869853
H, 1.512479, -0.076658, -2.868136
H, 1.880635, -1.674853, -3.537188
H, 1.042761, -0.803327, 0.317782
O, 1.634305, -0.706449, 1.098397
C, 1.346149, -1.781747, 2.001556
C, 1.779723, -3.12025, 1.431713
H, 0.275532, -1.7861, 2.228034
H, 1.886393, -1.557957, 2.921697
H, 2.853866, -3.121793, 1.230399
H, 1.250438, -3.329653, 0.498033
H, 1.558166, -3.924588, 2.138385
H, 3.36924, -0.676573, 0.601102

O, 4.30253, -0.606165, 0.30666
C, 4.486755, 0.69767, -0.2515
C, 4.345399, 1.788618, 0.795833
H, 3.775476, 0.855625, -1.068796
H, 5.490747, 0.707185, -0.677239
H, 5.084372, 1.652376, 1.589441
H, 3.348209, 1.76937, 1.243185
H, 4.499484, 2.772512, 0.34401

Linear-*gauche* $(EtOH)_7$

H, 5.796198, -1.185187, -1.553721
O, 4.97093, -0.681452, -1.619698
C, 3.88172, -1.599784, -1.830865
C, 3.775187, -2.615975, -0.711304
H, 2.987783, -0.979293, -1.882502
H, 4.015723, -2.093528, -2.795998
H, 3.634473, -2.119733, 0.251554
H, 4.67959, -3.228688, -0.661169
H, 2.924148, -3.278197, -0.889975
H, 4.644697, 0.360469, -0.187543
O, 4.382546, 0.940435, 0.560439
C, 3.941671, 2.201456, 0.032045
C, 2.793915, 2.034323, -0.947187
H, 4.786466, 2.706716, -0.443569
H, 3.635191, 2.792904, 0.894925
H, 1.973515, 1.481657, -0.484849
H, 3.1217, 1.495133, -1.83925
H, 2.419009, 3.013455, -1.258208
H, 3.110056, 0.146574, 1.493374
O, 2.412225, -0.302541, 2.023515
C, 1.971239, 0.587641, 3.060542
C, 0.954028, 1.595619, 2.556539
H, 2.841167, 1.094816, 3.485934
H, 1.534253, -0.040033, 3.837724
H, 0.070998, 1.090034, 2.158482
H, 1.380404, 2.22329, 1.770421
H, 0.63601, 2.244205, 3.377774
H, 1.252768, -0.756918, 0.766849
O, 0.650553, -1.04395, 0.04226
C, -0.054028, -2.213514, 0.482031
C, -0.964768, -1.913879, 1.658807
H, 0.669248, -2.990855, 0.744009
H, -0.628621, -2.561803, -0.376601
H, -1.683802, -1.132329, 1.402243
H, -0.381045, -1.582025, 2.521738
H, -1.516505, -2.813128, 1.945956
H, -0.370123, 0.34891, -0.340477
O, -0.872244, 1.132445, -0.663046
C, -0.815925, 1.122673, -2.096861
C, -1.664076, 0.010138, -2.685526
H, 0.22638, 1.020993, -2.412737
H, -1.173832, 2.098777, -2.424273
H, -2.708956, 0.119782, -2.385072
H, -1.30351, -0.966074, -2.350159
H, -1.614017, 0.035772, -3.777619
H, -2.482899, 1.048452, 0.081496
O, -3.352704, 1.035473, 0.542579
C, -3.899651, 2.361518, 0.510494
C, -4.218159, 2.806842, -0.905315
H, -3.195901, 3.052139, 0.983437
H, -4.80402, 2.328504, 1.118236
H, -4.928643, 2.121367, -1.374029
H, -3.310381, 2.839464, -1.513218
H, -4.658027, 3.807823, -0.89493
H, -4.449449, -0.134803, -0.28662
O, -4.963137, -0.842082, -0.731735
C, -4.3879, -2.093463, -0.346141
C, -4.720196, -2.448949, 1.092848
H, -3.30308, -2.061517, -0.493992
H, -4.795866, -2.841944, -1.026618
H, -5.803252, -2.503466, 1.228148
H, -4.322318, -1.697319, 1.779528
H, -4.28922, -3.418883, 1.356136

Linear-*gauche* $(EtOH)_8$

H, 5.564105, 3.072418, -0.469361
O, 4.898672, 2.603188, 0.05586
C, 3.595507, 2.883823, -0.488083
C, 3.488087, 2.471431, -1.942463
H, 2.897943, 2.31921, 0.129567
H, 3.381732, 3.947999, -0.365841
H, 3.706922, 1.407809, -2.061162
H, 4.186628, 3.044041, -2.558806
H, 2.475805, 2.661624, -2.308386
H, 5.188841, 0.832916, 0.217945
O, 5.275612, -0.135423, 0.356965
C, 5.034546, -0.420314, 1.743611
C, 3.64913, 0.020348, 2.180597
H, 5.803385, 0.067386, 2.348882
H, 5.15366, -1.498123, 1.851497
H, 2.883031, -0.424129, 1.5412
H, 3.557346, 1.108022, 2.133645
H, 3.462803, -0.292823, 3.211667
H, 4.156717, -0.957061, -0.745662
O, 3.530023, -1.362479, -1.388214
C, 3.550661, -2.788815, -1.232359

C, 2.847334, -3.237897, 0.035848
H, 4.588223, -3.132923, -1.241038
H, 3.053577, -3.196207, -2.112704
H, 1.810603, -2.892026, 0.047717
H, 3.354839, -2.849533, 0.922103
H, 2.846338, -4.329907, 0.094216
H, 2.020726, -0.530445, -1.018213
O, 1.218484, 0.005663, -0.820537
C, 0.334321, -0.055863, -1.947599
C, -0.171099, -1.465909, -2.193458
H, 0.851357, 0.327104, -2.831992
H, -0.493669, 0.616788, -1.720456
H, -0.684917, -1.85217, -1.310092
H, 0.658271, -2.135451, -2.437213
H, -0.87155, -1.471347, -3.032831
H, 0.430685, -0.461792, 0.672756
O, -0.04716, -0.646338, 1.51534
C, -0.239819, 0.59785, 2.204093
C, -1.018598, 1.595966, 1.365426
H, 0.733899, 1.008703, 2.48707
H, -0.779523, 0.352774, 3.11901
H, -1.958151, 1.156531, 1.023303
H, -0.439757, 1.904121, 0.491268
H, -1.244904, 2.487842, 1.95643
H, -1.574826, -1.43419, 1.098748
O, -2.406249, -1.896712, 0.84293
C, -3.182784, -2.149229, 2.023003
C, -3.903244, -0.903797, 2.507173
H, -2.528059, -2.546947, 2.802864
H, -3.898992, -2.926813, 1.756705
H, -4.566616, -0.516034, 1.729809
H, -3.189384, -0.123442, 2.782145
H, -4.50774, -1.139378, 3.387595
H, -3.131317, -0.804384, -0.356946
O, -3.476973, -0.235467, -1.081832
C, -4.136262, -1.080727, -2.03483
C, -5.363491, -1.750898, -1.443278
H, -3.430552, -1.830206, -2.403337
H, -4.411718, -0.43513, -2.86925
H, -6.075344, -1.004213, -1.083023
H, -5.084682, -2.399926, -0.608781
H, -5.858299, -2.364085, -2.201381
H, -4.667813, 1.002465, -0.485163
O, -5.324304, 1.673942, -0.201662
C, -4.622549, 2.739206, 0.444928
C, -3.681971, 3.45862, -0.506414
H, -4.073436, 2.351022, 1.308493
H, -5.385668, 3.423588, 0.817143
H, -4.242004, 3.893897, -1.337763
H, -2.939733, 2.767296, -0.914474
H, -3.15223, 4.261359, 0.014129

Cyclic-*gauche* $(EtOH)_3$

C, 2.378053, -2.515346, 0.070234
C, 0.956936, -2.18314, 0.482757
O, 0.201468, -1.6403, -0.610711
H, 0.621136, -0.798204, -0.879189
H, 2.379946, -3.243751, -0.74384
H, 2.902805, -1.616124, -0.26449
H, 2.927822, -2.937139, 0.915598
H, 0.423092, -3.079872, 0.795853
H, 0.952147, -1.474536, 1.316801
H, -1.167596, -0.563214, 0.234677
O, -1.51425, 0.293015, 0.555342
C, -2.687028, 0.619202, -0.205711
C, -3.833451, -0.3255, 0.101021
H, -2.445075, 0.60025, -1.272336
H, -2.94298, 1.642635, 0.067384
H, -4.081058, -0.295847, 1.16458
H, -3.569534, -1.351804, -0.167573
H, -4.72059, -0.040173, -0.470438
H, -0.006657, 1.130769, -0.268875
O, 0.804299, 1.126327, -0.816646
C, 1.904677, 1.574772, -0.013184
C, 1.755498, 3.033514, 0.375484
H, 2.797274, 1.426496, -0.620445
H, 1.988261, 0.946328, 0.878311
H, 0.858213, 3.181013, 0.98232
H, 1.681944, 3.661419, -0.515284
H, 2.620604, 3.358406, 0.959465

Cyclic-*gauche* $(EtOH)_4$

C, 1.775614, 3.500326, -0.970732
C, 0.440444, 2.781261, -1.005926
O, 0.27906, 1.920475, 0.131428
H, 0.941213, 1.194404, 0.061272
H, 1.863801, 4.098408, -0.060802
H, 2.599261, 2.78178, -0.998391
H, 1.870861, 4.163625, -1.834388
H, -0.385288, 3.491804, -0.965854
H, 0.342135, 2.192721, -1.92278
H, -1.194096, 0.94107, -0.060384
O, -1.920044, 0.278733, -0.130065
C, -2.781027, 0.440917, 1.007031
C, -3.501661, 1.775183, 0.969676
H, -2.192364, 0.344764, 1.92403
H, -3.49061, -0.385703, 0.968282

H, -4.099902, 1.861142, 0.059637
H, -2.78408, 2.599716, 0.995917
H, -4.165018, 1.871089, 1.833215
H, -0.94063, -1.194215, 0.061572
O, -0.278248, -1.920217, 0.129833
C, -0.441484, -2.77979, -1.008183
C, -1.774635, -3.502394, -0.969153
H, 0.386237, -3.488236, -0.97218
H, -0.348057, -2.189628, -1.924501
H, -2.600239, -2.785943, -0.992412
H, -1.857759, -4.102257, -0.059918
H, -1.871477, -4.164464, -1.833577
H, 1.194507, -0.940807, -0.062276
O, 1.920577, -0.27855, -0.131019
C, 2.780063, -0.441011, 1.007172
C, 3.501445, -1.774875, 0.969955
H, 2.190046, -0.345786, 1.923403
H, 3.489254, 0.38602, 0.969988
H, 4.101146, -1.859847, 0.060784
H, 2.784242, -2.599791, 0.994453
H, 4.163506, -1.871094, 1.834455

Cyclic-*gauche* $\left(\mathrm{EtOH}\right)_5$

C, 4.21055, 1.594339, -0.291827
C, 3.347474, 0.509163, 0.324029
O, 2.22699, 0.191995, -0.514859
H, 1.602352, 0.95309, -0.492105
H, 4.589159, 1.273613, -1.265058
H, 3.636741, 2.514751, -0.427917
H, 5.062309, 1.813876, 0.357451
H, 3.914171, -0.415476, 0.437026
H, 2.988171, 0.80914, 1.312459
H, 1.388171, -1.2519, 0.033023
O, 0.924142, -2.085524, 0.282518
C, 1.240527, -3.082649, -0.701683
C, 2.716012, -3.43395, -0.688867
H, 0.937136, -2.725734, -1.690142
H, 0.6333, -3.95345, -0.453769
H, 3.019692, -3.777597, 0.302813
H, 3.323218, -2.566926, -0.960925
H, 2.917982, -4.231149, -1.409124
H, -0.789427, -1.732105, 0.077725
O, -1.749313, -1.534938, -0.030243
C, -2.410677, -1.852602, 1.204001
C, -2.429472, -3.348244, 1.457297
H, -3.42465, -1.462036, 1.113038
H, -1.915445, -1.326535, 2.025176
H, -1.41179, -3.737136, 1.547135
H, -2.931962, -3.868945, 0.638795
H, -2.962244, -3.566764, 2.386529
H, -1.900673, 0.207776, -0.196585
O, -2.008245, 1.187428, -0.223485
C, -2.729639, 1.535045, -1.414768
C, -4.151036, 1.006873, -1.381287
H, -2.194971, 1.151271, -2.288204
H, -2.723189, 2.624353, -1.462829
H, -4.682116, 1.39213, -0.507812
H, -4.156965, -0.085536, -1.34295
H, -4.688477, 1.319275, -2.280601
H, -0.410033, 1.904588, -0.310291
O, 0.482694, 2.323413, -0.285264
C, 0.641694, 2.920793, 1.010569
C, -0.320995, 4.076266, 1.212852
H, 1.673945, 3.267142, 1.062093
H, 0.496769, 2.159284, 1.782595
H, -1.356165, 3.729852, 1.158261
H, -0.167823, 4.841402, 0.448189
H, -0.163951, 4.530555, 2.194775

Gauche-$\left[\mathrm{OAc}\left(\mathrm{EtOH}\right)\right]^-$

O, -1.115894, -0.588895, 1.115468
O, -0.917949, 0.897652, -0.545687
C, -1.565788, 0.02416, 0.11276
C, -2.981533, -0.269015, -0.357101
H, -3.419959, -1.10056, 0.192856
H, -3.595822, 0.622943, -0.209891
H, -2.977921, -0.493353, -1.425636
C, 2.314143, -0.05987, 0.442062
H, 1.844764, -0.497944, 1.32863
H, 3.356537, 0.150551, 0.686244
C, 2.230411, -1.026931, -0.727092
H, 2.733351, -1.965814, -0.478614
H, 1.188263, -1.251249, -0.969211
H, 2.709006, -0.600738, -1.612478
O, 1.711891, 1.200101, 0.145264
H, 0.754, 1.055233, -0.056035

Gauche-$\left[\mathrm{OAc}\left(\mathrm{EtOH}\right)_2\right]^-$

O, 0.113636, 0.484312, 0.038825
O, -1.384101, 1.963647, -0.709449
C, -0.269104, 1.676425, -0.215074
C, 0.717125, 2.784291, 0.106924
H, 1.007843, 2.723256, 1.157987

H, 1.620089, 2.64625, -0.49325
H, 0.290844, 3.764762, -0.09994
O, -1.591948, -1.590196, -0.540433
C, -2.953373, -1.197211, -0.357414
H, -3.196826, -0.37233, -1.034026
H, -3.560637, -2.057144, -0.64391
C, -3.242154, -0.801291, 1.080871
H, -4.296042, -0.533384, 1.197631
H, -3.016978, -1.629792, 1.757205
H, -2.635636, 0.060172, 1.372269
H, -1.015584, -0.811541, -0.35145
O, 2.649168, -0.006115, 0.920661
C, 3.188762, -0.735442, -0.183616
H, 3.020236, -0.177547, -1.111012
H, 4.265652, -0.795166, -0.019436
C, 2.590031, -2.127787, -0.289624
H, 2.775076, -2.69228, 0.627727
H, 1.510221, -2.071766, -0.451178
H, 3.034817, -2.671534, -1.127843
H, 1.715164, 0.21096, 0.689987

Gauche-$\left[\mathrm{OAc(EtOH)_3}\right]^-$

O, 0.177232, -0.595095, -0.163168
O, -1.360801, -1.511038, -1.492811
C, -0.319391, -1.585418, -0.788593
C, 0.409041, -2.910289, -0.697188
H, 1.239221, -2.893997, -1.409415
H, 0.823429, -3.053987, 0.301338
H, -0.251952, -3.73731, -0.953223
O, -0.008918, 1.856479, -1.462005
C, -0.324451, 2.877143, -0.512673
H, -0.386144, 3.808291, -1.077626
H, -1.308846, 2.685895, -0.074879
C, 0.729268, 2.988153, 0.576354
H, 0.461011, 3.77814, 1.283594
H, 0.816621, 2.048709, 1.129111
H, 1.703537, 3.22715, 0.143164
O, 2.361505, -0.82585, 1.475699
C, 3.492508, -0.877338, 0.60378
H, 4.35426, -1.107495, 1.23183
H, 3.371262, -1.697093, -0.112319
C, 3.706883, 0.435647, -0.129969
H, 2.847311, 0.669345, -0.763353
H, 3.846082, 1.252106, 0.583019
H, 4.594853, 0.374413, -0.765625
H, 1.555592, -0.755005, 0.913528
H, -0.012136, 0.990709, -0.997224
O, -3.057471, 0.425232, -0.409072
C, -2.908159, 0.385504, 1.011567
H, -1.890431, 0.676979, 1.289057
H, -3.592646, 1.136826, 1.408232
C, -3.235049, -0.982923, 1.585658
H, -2.545319, -1.739301, 1.201857
H, -3.150606, -0.965442, 2.675805
H, -4.254102, -1.275414, 1.320277
H, -2.417257, -0.204219, -0.809911

Gauche-$\left[\mathrm{OAc(EtOH)_4}\right]^-$

O, 1.059878, -0.312539, 0.463836
O, -1.065132, -0.570686, -0.150371
C, -0.041167, -0.933308, 0.501007
C, -0.157886, -2.174718, 1.35858
H, -0.374322, -3.032946, 0.717815
H, 0.756672, -2.360646, 1.919377
H, -0.995075, -2.059297, 2.050639
O, 1.435536, 1.630201, -1.470625
C, 2.009092, 2.695692, -0.71079
H, 1.986114, 3.578723, -1.350944
H, 1.385653, 2.900377, 0.165842
C, 3.434577, 2.38616, -0.285294
H, 3.861449, 3.233617, 0.25883
H, 3.462485, 1.511165, 0.369233
H, 4.059122, 2.186289, -1.159654
O, 3.41798, -1.551918, 1.163457
C, 3.645308, -2.34843, -0.002223
H, 4.456253, -3.034119, 0.247027
H, 2.753568, -2.946769, -0.218971
C, 4.018756, -1.501599, -1.206851
H, 3.206033, -0.819864, -1.469222
H, 4.913713, -0.910772, -0.995749
H, 4.221531, -2.141035, -2.070774
H, 2.579994, -1.061149, 1.015205
H, 1.247426, 0.89605, -0.845051
O, -1.658737, 2.127571, -0.334564
C, -2.447239, 2.209272, 0.855022
H, -3.020206, 3.134681, 0.78058
H, -3.156555, 1.375795, 0.888153
C, -1.585155, 2.219938, 2.105466
H, -0.893353, 3.065576, 2.085956
H, -2.210361, 2.304413, 2.998927
H, -1.002992, 1.297402, 2.180813
H, -1.305221, 1.213634, -0.38164
O, -3.482883, -1.829881, 0.243571
H, -2.609842, -1.385745, 0.150564
C, -4.117213, -1.811785, -1.037898
H, -4.992028, -2.458096, -0.955329

H, -3.447226, -2.246531, -1.786734
C, -4.530363, -0.409602, -1.450875
H, -3.657184, 0.242628, -1.533854
H, -5.032164, -0.433625, -2.422335
H, -5.218874, 0.018533, -0.718007

Gauche-$\left[\mathrm{OAc(EtOH)_5}\right]^-$

O, 1.581333, -0.428924, -0.035713
O, -0.460108, -0.154748, -0.881959
C, 0.421232, -0.857389, -0.306121
C, 0.09308, -2.28141, 0.089346
H, 0.803228, -2.958821, -0.390424
H, 0.212484, -2.389272, 1.170005
H, -0.921295, -2.556949, -0.194116
O, 2.640281, 1.805257, -1.287868
C, 3.111362, 2.636404, -0.224265
H, 3.437989, 3.568737, -0.687035
H, 2.28541, 2.869271, 0.454652
C, 4.257481, 1.994991, 0.540109
H, 4.608161, 2.667312, 1.328421
H, 3.937098, 1.059402, 1.006051
H, 5.093689, 1.781381, -0.130297
O, 3.439697, -2.134676, 1.078661
C, 4.129994, -2.690555, -0.042936
H, 4.753631, -3.494903, 0.349464
H, 3.409395, -3.13345, -0.738621
C, 4.984349, -1.657406, -0.757529
H, 4.36299, -0.854568, -1.162239
H, 5.712103, -1.221329, -0.068603
H, 5.52587, -2.12245, -1.586252
H, 2.763645, -1.510437, 0.731552
H, 2.206221, 1.0215, -0.884263
O, -0.589096, 2.552465, -0.261046
C, -1.332784, 2.466885, 0.956875
H, -1.760428, 3.456355, 1.125588
H, -2.160314, 1.760015, 0.835695
C, -0.456924, 2.063347, 2.131091
H, 0.348727, 2.788382, 2.270561
H, -1.047584, 2.02359, 3.050647
H, -0.011721, 1.078945, 1.963987
H, -0.396504, 1.635672, -0.551243
O, -2.931239, -1.149214, -1.499658
H, -2.039718, -0.802492, -1.256698
C, -3.50118, -0.29346, -2.498082
H, -4.417809, -0.7835, -2.827583
H, -2.820952, -0.234064, -3.35241
C, -3.798905, 1.092309, -1.95487
H, -2.879714, 1.586075, -1.630693
H, -4.262028, 1.708748, -2.730457
H, -4.485035, 1.032493, -1.106045
O, -4.591342, -1.535186, 0.694932
H, -3.992078, -1.375828, -0.066624
C, -4.204224, -0.667093, 1.762966
H, -4.911975, -0.84967, 2.572385
H, -4.313224, 0.377369, 1.451995
C, -2.783231, -0.934303, 2.228514
H, -2.671414, -1.979351, 2.52921
H, -2.068151, -0.72317, 1.430114
H, -2.538394, -0.298694, 3.083889

Gauche-$\left[\mathrm{OAc(EtOH)_6}\right]^-$

O, 0.652543, 0.157958, -0.985342
O, -1.552813, 0.43329, -1.11586
C, -0.516445, -0.28971, -1.17807
C, -0.656666, -1.763679, -1.492796
H, -0.047013, -2.004376, -2.366509
H, -0.27365, -2.347339, -0.652478
H, -1.692685, -2.039008, -1.683454
O, 1.314853, 2.858345, -1.090888
C, 1.845073, 3.232795, 0.1833
H, 2.128668, 4.282677, 0.098151
H, 1.063925, 3.156025, 0.944923
C, 3.045511, 2.386912, 0.572361
H, 3.428224, 2.69928, 1.54851
H, 2.767096, 1.331968, 0.638134
H, 3.845573, 2.494449, -0.164093
O, 2.750659, -1.570587, -0.785446
C, 3.461637, -1.496023, -2.026662
H, 4.224404, -2.274441, -1.990522
H, 2.778599, -1.732753, -2.8481
C, 4.090991, -0.130857, -2.239322
H, 3.322745, 0.645934, -2.269628
H, 4.790724, 0.102113, -1.433065
H, 4.6365, -0.110144, -3.186935
H, 1.979472, -0.955694, -0.837164
H, 1.00563, 1.927965, -1.032378
O, -1.645422, 2.416266, 0.833367
C, -1.944813, 1.601147, 1.96908
H, -2.366602, 2.267483, 2.723021
H, -2.712795, 0.867077, 1.703743
C, -0.707376, 0.905018, 2.510681
H, 0.043474, 1.640753, 2.809697
H, -0.961446, 0.298677, 3.384646
H, -0.266148, 0.25097, 1.753993
H, -1.494697, 1.815411, 0.073199
O, -4.065027, -0.587379, -1.461464

H, -3.148725, -0.250006, -1.319635
C, -4.929973, 0.52913, -1.706391
H, -5.880365, 0.109232, -2.036875
H, -4.52039, 1.127877, -2.524632
C, -5.121314, 1.379698, -0.463612
H, -4.169052, 1.800855, -0.133024
H, -5.804472, 2.207293, -0.67429
H, -5.543491, 0.782285, 0.348662
O, -4.938301, -2.307313, 0.533703
H, -4.617255, -1.68208, -0.152237
C, -4.266551, -2.016255, 1.761397
H, -4.689531, -2.692517, 2.505118
H, -4.4919, -0.991543, 2.075444
C, -2.764675, -2.218322, 1.653343
H, -2.539735, -3.238318, 1.331046
H, -2.330479, -1.521634, 0.932424
H, -2.288041, -2.048334, 2.622728
O, 3.958988, -1.181835, 1.705212
H, 3.575624, -1.309422, 0.811228
C, 5.268634, -0.628142, 1.562457
H, 5.221146, 0.30013, 0.984384
H, 5.602957, -0.375935, 2.569545
C, 6.229569, -1.610267, 0.915194
H, 5.888676, -1.881383, -0.087734
H, 7.226792, -1.169769, 0.829486
H, 6.30279, -2.522392, 1.512649

Trans-$\left[\mathrm{OAc(EtOH)}\right]^-$

O, 1.891036, 1.33454, 0.169822
O, 0.9545, -0.637419, -0.321043
C, 1.949488, 0.090665, -0.008924
C, 3.285281, -0.616485, 0.148811
H, 4.076795, 0.081207, 0.418862
H, 3.199941, -1.387381, 0.918153
H, 3.543961, -1.115347, -0.788079
C, -2.289041, -0.47344, 0.168563
H, -1.961022, -0.693386, 1.189985
H, -2.178282, -1.387115, -0.424971
C, -3.734616, -0.021703, 0.169047
H, -4.376528, -0.797756, 0.592967
H, -3.850303, 0.886554, 0.765579
H, -4.0707, 0.186577, -0.849708
O, -1.483206, 0.566774, -0.386171
H, -0.549175, 0.241264, -0.388625

Trans-$\left[\mathrm{OAc(EtOH)_2}\right]^-$

O, -0.076991, 0.811402, -0.216512
O, 1.472871, 2.420805, -0.174045
C, 0.290397, 2.025226, -0.056548
C, -0.80356, 3.016211, 0.296792
H, -1.573125, 2.999399, -0.478733
H, -1.276131, 2.714922, 1.234734
H, -0.407919, 4.025728, 0.396633
O, 1.873766, -1.032191, -0.736927
C, 2.705911, -1.034101, 0.424225
H, 3.122315, -0.034536, 0.583764
H, 2.112687, -1.298067, 1.306367
C, 3.820847, -2.038382, 0.221968
H, 4.474665, -2.060947, 1.097258
H, 3.411497, -3.040326, 0.070488
H, 4.421555, -1.772346, -0.651307
H, 1.1763, -0.346615, -0.603733
O, -2.665771, 0.00503, 0.016306
C, -2.49536, -1.414388, 0.019627
H, -1.950511, -1.724149, -0.878
H, -1.906926, -1.715148, 0.892875
C, -3.860859, -2.068735, 0.056503
H, -4.407184, -1.765083, 0.952952
H, -4.446185, -1.783631, -0.821248
H, -3.760272, -3.156719, 0.065746
H, -1.766025, 0.402158, -0.053783

Trans-$\left[\mathrm{OAc(EtOH)_3}\right]^-$

O, 0.009447, 1.01477, 0.145983
O, 1.522413, 2.308794, -0.863451
C, 0.416138, 2.139593, -0.287283
C, -0.500692, 3.328586, -0.082005
H, -1.441501, 3.155049, -0.61033
H, -0.732581, 3.42815, 0.980703
H, -0.045026, 4.248117, -0.445348
O, -0.138505, -1.417301, -1.155543
C, -0.434661, -2.245851, -0.027891
H, 0.492321, -2.50817, 0.493479
H, -1.073647, -1.701007, 0.673329
C, -1.133505, -3.49859, -0.513631
H, -1.349086, -4.161836, 0.327541
H, -2.075848, -3.246206, -1.00664
H, -0.502812, -4.038031, -1.224712
O, -2.526563, 0.678786, 1.118233
C, -3.277939, 0.325676, -0.046025

H, -3.535085, 1.2285, -0.610571
H, -2.674353, -0.316341, -0.694259
C, -4.536699, -0.397722, 0.38569
H, -4.284543, -1.317099, 0.920492
H, -5.136148, 0.235297, 1.044957
H, -5.143263, -0.657919, -0.485205
H, -1.604854, 0.875178, 0.831698
H, 0.0598, -0.520176, -0.813742
O, 3.569722, 0.650546, 0.020489
C, 3.123167, -0.668211, 0.345139
H, 2.372139, -0.622613, 1.139609
H, 2.664228, -1.131398, -0.533333
C, 4.319301, -1.476973, 0.801023
H, 4.776326, -1.022582, 1.683626
H, 4.014341, -2.4949, 1.05607
H, 5.070069, -1.529503, 0.008768
H, 2.806751, 1.17368, -0.311919

Trans-$\left[\mathrm{OAc(EtOH)_4}\right]^-$

O, 0.484046, -0.718852, -0.160561
O, -1.528249, -0.479526, -1.085743
C, -0.653749, -1.167761, -0.479372
C, -1.008113, -2.585276, -0.086508
H, -1.633268, -3.049604, -0.849293
H, -0.112151, -3.181886, 0.082349
H, -1.582192, -2.548827, 0.844219
O, 2.202756, 1.078882, -1.374112
C, 2.939241, 1.568814, -0.250089
H, 2.47193, 2.484405, 0.127933
H, 2.923907, 0.826004, 0.552593
C, 4.363246, 1.853098, -0.682076
H, 4.941652, 2.248513, 0.156634
H, 4.847669, 0.940966, -1.039742
H, 4.376299, 2.591828, -1.487549
O, -4.156355, -1.262139, -0.811883
H, -3.21421, -1.048859, -0.992752
C, -4.612584, -0.361429, 0.201354
H, -3.952084, -0.419113, 1.072639
H, -4.588281, 0.665708, -0.176104
C, -6.02574, -0.745667, 0.585997
H, -6.052456, -1.765343, 0.977928
H, -6.407567, -0.069037, 1.354208
H, -6.686845, -0.689407, -0.282374
O, 2.513814, -1.950553, 1.204165
C, 3.514855, -2.109524, 0.194265
H, 3.409855, -3.092655, -0.276865
H, 3.379161, -1.350492, -0.581086
C, 4.883942, -1.97605, 0.828836
H, 5.005673, -0.985275, 1.274444
H, 5.018329, -2.726464, 1.612097
H, 5.666079, -2.117973, 0.078703
H, 1.704124, -1.599985, 0.772046
H, 1.462236, 0.533775, -1.035567
O, -1.861242, 1.994758, 0.186989
C, -0.584499, 2.610227, 0.386279
H, 0.03591, 1.976227, 1.02691
H, -0.076874, 2.726174, -0.575731
C, -0.799387, 3.961717, 1.034136
H, -1.303461, 3.850195, 1.99724
H, 0.160352, 4.456427, 1.202631
H, -1.410541, 4.601926, 0.393238
H, -1.724684, 1.153328, -0.296528

Trans-$\left[\mathrm{OAc(EtOH)_5}\right]^-$

O, -0.86362, -0.234995, 0.184606
O, 1.187768, -1.096996, 0.06227
C, -0.032894, -1.077195, -0.267237
C, -0.520322, -2.138865, -1.229467
H, -0.602029, -3.083268, -0.68411
H, -1.495257, -1.886238, -1.644593
H, 0.203865, -2.280108, -2.033157
O, 0.115568, 2.336159, 0.408172
C, 0.789733, 2.415861, -0.850035
H, 1.615532, 1.697264, -0.876206
H, 0.097055, 2.163052, -1.660251
C, 1.313996, 3.825236, -1.028127
H, 1.840779, 3.91601, -1.98102
H, 0.492095, 4.545514, -1.017527
H, 2.008758, 4.080027, -0.223892
O, -4.828423, -1.272047, 0.136748
H, -4.280591, -0.69037, -0.431918
C, -4.032564, -1.649947, 1.265563
H, -3.155902, -2.212937, 0.930149
H, -3.681742, -0.7542, 1.787649
C, -4.881523, -2.499492, 2.186995
H, -5.22374, -3.399335, 1.670097
H, -4.303266, -2.803518, 3.06258
H, -5.755885, -1.939172, 2.526964
O, -3.093495, 0.440594, -1.222549
C, -3.427789, 1.760607, -0.770334
H, -3.504846, 1.764712, 0.321366
H, -2.634446, 2.455473, -1.059673
C, -4.743831, 2.16309, -1.40046
H, -4.664168, 2.156315, -2.490186
H, -5.538546, 1.474058, -1.104025
H, -5.023044, 3.169861, -1.081085

H, -2.268936, 0.157408, -0.760121
H, -0.224181, 1.420245, 0.49689
O, 2.548264, 0.068875, 2.177907
C, 3.313419, 1.187536, 1.722694
H, 3.8486, 0.92405, 0.805028
H, 2.649028, 2.027749, 1.502284
C, 4.294888, 1.570036, 2.810726
H, 4.968438, 0.738292, 3.031245
H, 4.895085, 2.427287, 2.496301
H, 3.763452, 1.839876, 3.726596
H, 1.990293, -0.259718, 1.440851
O, 3.146502, -2.508843, -1.237271
H, 2.359926, -2.124276, -0.791192
C, 4.218965, -1.579767, -1.060579
H, 3.922426, -0.596336, -1.440067
H, 4.448607, -1.478661, 0.0053
C, 5.431035, -2.088177, -1.812774
H, 5.211308, -2.175486, -2.879556
H, 6.270122, -1.399578, -1.687743
H, 5.732012, -3.069493, -1.437839

Trans-$\left[\mathrm{OAc(EtOH)_6}\right]^-$

O, -1.003886, -0.343632, -1.201943
O, 0.829629, 0.884235, -0.888067
C, -0.405356, 0.67007, -0.730378
C, -1.220154, 1.656658, 0.078058
H, -2.128781, 1.918432, -0.467114
H, -1.517397, 1.178987, 1.015898
H, -0.648257, 2.556158, 0.30147
O, -0.219018, -2.756856, -0.044489
C, -0.060786, -2.241223, 1.280807
H, 0.641517, -1.401409, 1.270509
H, -1.023361, -1.875729, 1.654239
C, 0.460228, -3.351247, 2.169196
H, 0.580315, -2.991201, 3.193633
H, -0.238626, -4.191306, 2.179997
H, 1.428535, -3.709007, 1.810439
O, -5.050674, 1.35346, -0.657169
H, -4.484075, 0.562566, -0.527403
C, -5.253551, 1.955322, 0.624205
H, -5.694315, 1.225089, 1.310733
H, -4.29275, 2.274614, 1.04108
C, -6.174804, 3.144825, 0.456997
H, -7.141506, 2.827484, 0.058479
H, -6.340803, 3.634129, 1.419657
H, -5.737287, 3.87362, -0.2297
O, -3.445705, -0.835158, -0.073767
C, -3.957453, -2.067726, -0.598381
H, -4.044749, -1.993963, -1.68627
H, -3.262561, -2.878474, -0.363069
C, -5.310579, -2.329415, 0.027743
H, -5.222347, -2.394943, 1.114915
H, -6.01044, -1.526927, -0.21832
H, -5.721538, -3.271332, -0.34285
H, -2.572544, -0.648647, -0.495279
H, -0.444982, -2.000048, -0.621198
O, 2.794644, -0.588293, -2.162749
C, 2.748413, -1.960598, -1.764955
H, 2.593013, -2.031052, -0.684151
H, 1.910725, -2.462525, -2.259532
C, 4.05649, -2.618463, -2.151841
H, 4.893916, -2.140891, -1.636753
H, 4.042189, -3.677295, -1.88227
H, 4.220546, -2.540056, -3.229485
H, 2.025106, -0.122393, -1.770042
O, 2.3607, 2.815654, 0.284042
H, 1.713519, 2.165725, -0.077635
C, 3.368755, 3.021189, -0.717
H, 3.833559, 2.063762, -0.970473
H, 2.903851, 3.425213, -1.620592
C, 4.400165, 3.984103, -0.170415
H, 4.872066, 3.57439, 0.726187
H, 5.17769, 4.165511, -0.916096
H, 3.936327, 4.939716, 0.085144
O, 3.556603, 1.120186, 2.160587
H, 3.158463, 1.820466, 1.602463
C, 3.607445, -0.072456, 1.368976
H, 2.649464, -0.214879, 0.864028
H, 4.384499, 0.023845, 0.603439
C, 3.910233, -1.245572, 2.276902
H, 3.123612, -1.368078, 3.025569
H, 3.984225, -2.167471, 1.694536
H, 4.860549, -1.091644, 2.794776

$\left[\mathrm{Zn(EtOH)_4}\right]^{2+}\left(\mathrm{EtOH}\right)$

Zn, 0.459271, 0.401758, -0.315951
O, -1.205625, 1.48226, -0.673547
O, 0.093321, -0.52379, 1.501464
O, 2.497443, 0.755481, -0.117096
H, 2.860288, 1.176026, -0.914092
O, 0.405082, -1.07739, -1.73073
H, -0.875945, -0.41198, 1.63049
H, -0.050838, -0.79661, -2.540732
H, -1.865556, 1.101684, -0.047633
C, -1.159091, 2.925206, -0.503071
H, -0.355528, 3.267854, -1.151693

H, -0.899521, 3.144385, 0.533475
C, 2.931218, 1.499821, 1.056425
H, 2.453885, 2.480171, 1.041652
H, 2.557313, 0.930796, 1.904279
C, 1.570905, -1.87546, -2.07692
H, 2.234285, -1.26901, -2.693746
H, 2.05956, -2.08951, -1.129328
C, 0.448008, -1.9278, 1.586408
H, 1.50905, -1.97223, 1.346785
H, -0.110989, -2.48258, 0.83096
C, 0.177431, -2.45484, 2.978092
H, 0.471437, -3.50529, 3.037274
H, 0.747126, -1.89193, 3.720208
H, -0.885907, -2.38422, 3.220548
C, 1.147371, -3.14358, -2.782485
H, 0.623605, -2.91435, -3.713688
H, 2.031471, -3.73768, -3.025158
H, 0.492669, -3.74016, -2.143948
C, 4.438216, 1.612943, 1.07755
H, 4.797255, 2.158617, 0.201302
H, 4.750083, 2.159505, 1.97033
H, 4.900314, 0.624166, 1.0948
C, -2.486383, 3.53848, -0.886914
H, -2.436343, 4.623235, -0.767365
H, -2.72859, 3.313142, -1.927278
H, -3.287194, 3.160809, -0.246399
O, -2.578883, -0.02182, 1.164435
C, -3.109399, -1.20926, 0.529765
H, -2.40037, -1.44543, -0.263772
H, -3.109559, -2.02337, 1.256687
C, -4.49602, -0.96406, -0.024152
H, -4.482605, -0.15442, -0.757152
H, -4.864183, -1.86971, -0.511813
H, -5.189946, -0.70295, 0.778776
H, -3.187634, 0.271647, 1.860369

$\left[\mathrm{Zn(EtOH)_4}\right]^{2+}\mathrm{(EtOH)_2}$

Zn, 0.030411, 0.185417, -0.11279
O, 1.547705, 1.29523, 0.732181
O, 1.137306, -0.973197, -1.416988
O, -1.420637, 1.626448, -0.407934
H, -2.310542, 1.292595, -0.15324
O, -1.221556, -1.171549, 0.804187
H, 2.080186, -0.712933, -1.293319
H, -2.135561, -0.814944, 0.874256
H, 2.37388, 1.113378, 0.228872
C, 1.430802, 2.705029, 1.040801
H, 0.470989, 2.818378, 1.539918
H, 1.415243, 3.270957, 0.107948
C, -1.497808, 2.496897, -1.560076
H, -0.4676, 2.691435, -1.852714
H, -1.998745, 1.963905, -2.369568
C, -0.799304, -1.755755, 2.062302
H, 0.281571, -1.866061, 1.987354
H, -1.02494, -1.053701, 2.865829
C, 0.998151, -2.416261, -1.388529
H, -0.047761, -2.611503, -1.615531
H, 1.214281, -2.775078, -0.38108
C, 1.914528, -3.048339, -2.411659
H, 1.785405, -4.132941, -2.399778
H, 1.683633, -2.681567, -3.41378
H, 2.96129, -2.826732, -2.18706
C, -1.475554, -3.090691, 2.278163
H, -1.240733, -3.775801, 1.460571
H, -1.126304, -3.532939, 3.214235
H, -2.559703, -2.971113, 2.338705
C, -2.221489, 3.775576, -1.200681
H, -1.703916, 4.29556, -0.391581
H, -2.261134, 4.436302, -2.069959
H, -3.246292, 3.563523, -0.885807
C, 2.575166, 3.132409, 1.932635
H, 2.478955, 4.19328, 2.175233
H, 2.5717, 2.560582, 2.862877
H, 3.534069, 2.982993, 1.429613
O, 3.536394, 0.230587, -0.836583
C, 4.609698, -0.459226, -0.152128
H, 5.138116, -1.084394, -0.872919
H, 5.300185, 0.283787, 0.24918
C, 3.998946, -1.291779, 0.951269
H, 3.294849, -2.021109, 0.542976
H, 4.786695, -1.834836, 1.47761
H, 3.477628, -0.659319, 1.673458
H, 3.90145, 0.753382, -1.566956
O, -3.57746, 0.212237, 0.490225
H, -4.127511, 0.542258, 1.217549
C, -4.425786, -0.334606, -0.545892
H, -5.104313, 0.447529, -0.889626
C, -5.181848, -1.549434, -0.052663
H, -5.802614, -1.95057, -0.857403
H, -4.489125, -2.329194, 0.271506
H, -5.834667, -1.286667, 0.783353
H, -3.748029, -0.591922, -1.358972

$\left[\mathrm{Zn(EtOH)_5}\right]^{2+}\mathrm{(EtOH)}$

Zn, -0.453142, 0.226843, -0.094591
O, -1.721504, 0.288639, 1.617856
O, -0.499984, 2.077529, -1.034893

O, -2.177903, -0.45905, -1.166199
O, 0.43965, -1.544595, -0.681532
O, 1.279858, 0.759802, 0.950467
H, -1.347883, 0.815593, 2.342123
H, -1.935159, -0.675528, -2.081107
C, 0.511534, 3.118465, -1.033791
C, -2.041712, -1.038817, 2.117285
C, -3.422349, 0.2831, -1.169399
C, -0.14495, -2.852397, -0.447455
C, 1.309688, 1.663202, 2.075622
H, -3.283194, 1.204966, -1.736825
H, -1.179854, -2.777207, -0.769605
H, 0.53554, 2.403957, 1.88089
H, -1.123036, -1.507873, 2.472176
H, -3.60738, 0.531736, -0.127204
H, 1.047615, 1.109693, 2.979897
C, -4.54072, -0.556827, -1.745797
H, -5.474666, 0.00947, -1.719694
H, -4.330652, -0.821319, -2.785196
H, -4.67212, -1.472954, -1.166246
C, 2.6726, 2.308112, 2.202816
H, 2.67714, 3.002332, 3.046451
H, 3.441576, 1.551721, 2.378911
H, 2.924963, 2.86154, 1.295796
C, 0.41841, 3.94189, -2.299074
H, -0.553116, 4.437515, -2.372062
H, 1.193265, 4.712592, -2.289148
C, 0.603876, -3.907808, -1.231272
H, 1.645723, -3.967128, -0.906508
H, 0.139673, -4.883438, -1.067233
C, -3.087623, -0.966581, 3.207227
H, -3.337663, -1.977293, 3.538598
H, -2.71684, -0.406113, 4.069126
H, -3.996973, -0.488822, 2.837369
H, -2.40989, -1.582729, 1.249863
H, 0.578227, -3.685863, -2.300138
H, 0.563336, 3.314022, -3.180676
H, 1.376001, -1.567919, -0.381967
H, 0.376227, 3.732878, -0.143239
H, 1.460478, 2.593512, -0.965058
H, -0.118968, -3.060808, 0.623075
H, -1.381722, 2.479172, -1.081864
H, 1.941479, 0.042649, 1.055459
O, 2.972517, -1.309051, 0.437269
H, 3.332459, -1.972946, 1.045478
C, 4.04696, -0.726291, -0.335026
H, 3.571351, 0.0378, -0.948631
H, 4.745541, -0.24076, 0.348311
C, 4.74179, -1.765593, -1.187477
H, 5.537663, -1.293011, -1.768132
H, 5.191001, -2.540626, -0.561621
H, 4.03801, -2.233037, -1.879347

$\left[\mathrm{Zn(EtOH)_5}\right]^{2+}\mathrm{(EtOH)_2}$

Zn, -0.096503, -0.174137, -0.099109
O, -1.231932, -1.923241, -0.569981
O, -1.612137, 1.053895, -0.778196
O, 1.12903, 1.554274, -0.001378
O, 1.620078, -1.233428, -0.610832
O, -0.488092, -0.579835, 1.909121
H, -2.161026, -1.678587, -0.369929
H, 2.075955, 1.447698, -0.231689
C, -1.525071, 1.761987, -2.036875
C, -1.185002, -2.418355, -1.929485
C, 0.861621, 2.872369, 0.518415
C, 1.986431, -2.503975, -0.027602
C, 0.081323, 0.312713, 2.902919
H, 1.288472, 2.946273, 1.520479
H, 2.610427, -3.034758, -0.748375
H, 1.161512, 0.358938, 2.757499
H, -0.132224, -2.58831, -2.145218
H, -0.221598, 2.948151, 0.591696
H, -0.350884, 1.286687, 2.684442
C, 1.429602, 3.940746, -0.392282
H, 1.205756, 4.9289, 0.016557
H, 2.515801, 3.844355, -0.470993
H, 0.996669, 3.871817, -1.392329
C, -0.272588, -0.149723, 4.297717
H, 0.143966, 0.546529, 5.029195
H, -1.355735, -0.187615, 4.429966
H, 0.14424, -1.140592, 4.495813
C, -2.584786, 2.839969, -2.106196
H, -2.463327, 3.553175, -1.287744
H, -2.500815, 3.379852, -3.05242
C, 2.704788, -2.324834, 1.293425
H, 2.078588, -1.790809, 2.012502
H, 2.951434, -3.303886, 1.711677
C, -1.987548, -3.694574, -2.056462
H, -1.931356, -4.066987, -3.082134
H, -1.595942, -4.462002, -1.385378
H, -3.038597, -3.516773, -1.814978
H, -1.562167, -1.642861, -2.600266
H, 3.635941, -1.769409, 1.158658
H, -3.585801, 2.404971, -2.048582
H, 2.420554, -0.683353, -0.764663
H, -0.523485, 2.1847, -2.068778
H, -1.630788, 1.044171, -2.852266

H, 1.054631, -3.052523, 0.095367
H, -2.467562, 0.570317, -0.720506
H, -0.238963, -1.497081, 2.111614
O, 3.566751, 0.681645, -0.954821
C, 4.801115, 0.666437, -0.204823
H, 5.239519, 1.665053, -0.235263
H, 4.509388, 0.445623, 0.82052
C, 5.757545, -0.372934, -0.747174
H, 6.02828, -0.143808, -1.781074
H, 6.672619, -0.384438, -0.15007
H, 5.309277, -1.368674, -0.714645
H, 3.752462, 0.919374, -1.876732
O, -3.697826, -0.644453, -0.260822
H, -4.438971, -0.739242, -0.87905
C, -4.209401, -0.328798, 1.055155
H, -3.349364, -0.398594, 1.719132
H, -4.933209, -1.093329, 1.339957
C, -4.820562, 1.055707, 1.093066
H, -5.660004, 1.12844, 0.39704
H, -5.191251, 1.267204, 2.099151
H, -4.079123, 1.814243, 0.831582

$\left[\mathrm{Zn(EtOH)_6}\right]^{2+}\mathrm{(EtOH)}$

Zn, 0.430497, 0.054959, 0.184173
O, -1.228728, 1.182228, -0.560743
O, -1.086894, -1.217248, 0.955814
O, 0.453397, 0.946787, 2.129154
O, 1.992688, -1.270454, 0.896151
O, 1.907251, 1.566158, -0.220614
O, 0.743523, -0.874277, -1.726519
C, 0.377349, -2.273283, -1.842448
H, -0.69917, -2.369759, -1.694108
H, 0.891341, -2.771966, -1.023399
C, -0.828374, -2.360162, 1.799326
H, -0.113718, -2.018558, 2.546795
H, -0.360559, -3.146215, 1.204278
C, -1.00045, 2.196528, -1.565288
H, -0.659751, 1.718783, -2.48711
H, -0.196068, 2.816782, -1.176016
C, -0.165331, 2.248865, 2.296065
H, -1.248541, 2.124513, 2.285392
H, 0.131631, 2.822281, 1.420892
C, 2.586451, 1.720191, -1.491541
H, 1.79988, 1.715667, -2.24247
H, 3.233349, 0.857998, -1.656219
C, 3.269339, -1.417489, 0.229448
H, 3.833363, -0.489447, 0.339809
H, 3.031928, -1.563204, -0.821376
C, -2.251772, 3.013613, -1.809002
H, -2.599696, 3.471345, -0.880366
H, -2.034713, 3.808836, -2.526307
H, -3.050805, 2.392831, -2.22048
C, 4.030914, -2.597283, 0.793829
H, 3.460117, -3.520166, 0.671292
H, 4.983525, -2.705029, 0.26965
H, 4.241694, -2.450396, 1.856202
C, 0.310343, 2.90318, 3.57392
H, -0.155164, 3.886196, 3.679148
H, 0.037213, 2.30183, 4.444476
H, 1.394461, 3.033331, 3.559944
C, 0.803865, -2.828798, -3.18286
H, 0.545236, -3.888871, -3.237865
H, 0.294304, -2.311046, -3.999401
H, 1.88252, -2.726804, -3.318563
C, 3.368431, 3.014843, -1.524811
H, 3.854068, 3.124958, -2.497369
H, 2.708368, 3.870166, -1.36639
H, 4.143977, 3.020069, -0.754726
C, -2.108588, -2.844555, 2.44612
H, -1.893421, -3.699108, 3.092136
H, -2.559314, -2.05609, 3.052324
H, -2.829118, -3.163842, 1.688487
H, -1.937847, 0.566595, -0.851938
H, 0.294061, -0.377508, -2.428402
H, 2.150863, -1.10941, 1.840324
H, 0.068513, 0.336871, 2.778518
H, -1.744986, -1.44025, 0.266126
H, 2.567246, 1.536676, 0.491119
O, -3.055723, -0.875476, -0.934445
C, -4.277291, -0.754219, -0.169055
H, -4.816309, -1.701292, -0.223328
H, -3.955446, -0.594058, 0.859183
C, -5.129839, 0.397537, -0.657418
H, -6.055955, 0.439401, -0.078349
H, -4.604581, 1.34677, -0.535599
H, -5.391457, 0.268584, -1.710786
H, -3.270363, -1.181785, -1.828824

$\left[\mathrm{Zn(EtOH)_6}\right]^{2+}\mathrm{(EtOH)_2}$

Zn, 0.097686, 0.114313, -0.044701
O, -1.226428, 1.497361, 0.898702
O, -1.359559, -1.392672, 0.395016
O, 1.322361, -0.158589, 1.733692
O, 1.393628, -1.494466, -0.667385
O, 1.528339, 1.661387, -0.396116
O, -0.791301, 0.133526, -2.006595

C, -2.222948, 0.258539, -2.184998
H, -2.533303, 1.2554, -1.867153
H, -2.658954, -0.481856, -1.519568
C, -1.030411, -2.45889, 1.312366
H, -0.924458, -2.044542, 2.318089
H, -0.065353, -2.842052, 0.986314
C, -1.14792, 2.915052, 1.143379
H, -0.118032, 3.198011, 0.938155
H, -1.354251, 3.092488, 2.200766
C, 0.981844, 0.564317, 2.938344
H, -0.043063, 0.318501, 3.222783
H, 1.02468, 1.615656, 2.661258
C, 1.371641, 2.577533, -1.500485
H, 0.325164, 2.880857, -1.493227
H, 1.580772, 2.047836, -2.433632
C, 1.06834, -2.390991, -1.749469
H, 1.19944, -1.868398, -2.698854
H, 0.013008, -2.629115, -1.629697
C, -2.11947, 3.674387, 0.263532
H, -3.146593, 3.352415, 0.456444
H, -2.053269, 4.744601, 0.475133
H, -1.893648, 3.515949, -0.793142
C, 1.923258, -3.639018, -1.685397
H, 1.781743, -4.156101, -0.733524
H, 1.646168, -4.319066, -2.494787
H, 2.982112, -3.391461, -1.795995
C, 1.953435, 0.247683, 4.054545
H, 1.680286, 0.812808, 4.94895
H, 1.925512, -0.816523, 4.303557
H, 2.973266, 0.517125, 3.772172
C, -2.607447, -0.009836, -3.62379
H, -3.692258, 0.063679, -3.733102
H, -2.147804, 0.721228, -4.293657
H, -2.295299, -1.011748, -3.925844
C, 2.289426, 3.770822, -1.335336
H, 2.152121, 4.465137, -2.167685
H, 2.071068, 4.297613, -0.403726
H, 3.335093, 3.453405, -1.322228
C, -2.088181, -3.542446, 1.277277
H, -1.799782, -4.361596, 1.940447
H, -3.054034, -3.157425, 1.613066
H, -2.199521, -3.938323, 0.265276
H, -2.120983, 1.163144, 1.115643
H, -0.350163, 0.77596, -2.584871
H, 2.29108, -1.119865, -0.800027
H, 1.364226, -1.107683, 1.931489
H, -2.210025, -0.988776, 0.677461
H, 2.390839, 1.19921, -0.491535
O, 3.720908, 0.026957, -0.827811
H, 4.174629, 0.149224, -1.676092
O, -3.554474, 0.043055, 1.302243
H, -3.784365, -0.272066, 2.189828
C, 4.705308, -0.096347, 0.224239
H, 5.323273, 0.802991, 0.23014
H, 4.130698, -0.131006, 1.147822
C, 5.54538, -1.343987, 0.051646
H, 6.091731, -1.315605, -0.89448
H, 6.273761, -1.413096, 0.863333
H, 4.918632, -2.238342, 0.071402
C, -4.755695, 0.13343, 0.502531
H, -4.484509, 0.7333, -0.364149
H, -5.51355, 0.672099, 1.072774
C, -5.246013, -1.237876, 0.088311
H, -5.515284, -1.835522, 0.962563
H, -6.133907, -1.135691, -0.540951
H, -4.478541, -1.768851, -0.48006

$\left[\mathrm{Zn(OAc)(EtOH)_2}\right]^+$

Zn, 0.026058, -0.219021, 0.021722
O, -0.605502, 1.5534, 0.940779
O, 0.495138, 1.657901, -0.953983
O, -1.606254, -1.331532, -0.401637
O, 1.738826, -1.238827, 0.387811
C, -0.111694, 2.245253, -0.007956
C, -0.279161, 3.73511, -0.001809
H, 0.389191, 4.205175, -0.719754
H, -1.313975, 3.963423, -0.270256
H, -0.099947, 4.124926, 1.000253
C, 2.98259, -0.640445, -0.08578
C, 4.100335, -1.655649, -0.04248
H, 3.864493, -2.516538, -0.670728
H, 5.020979, -1.197344, -0.41113
H, 4.276122, -1.997983, 0.980076
H, 2.770042, -0.320781, -1.10303
H, 3.198112, 0.234459, 0.527559
H, 1.833074, -1.484588, 1.322618
C, -2.886784, -0.86798, 0.112874
C, -3.930296, -1.951763, -0.025263
H, -4.875705, -1.598505, 0.393066
H, -4.095576, -2.202395, -1.075908
H, -3.625741, -2.851881, 0.511886
H, -2.697988, -0.62465, 1.155661
H, -3.167667, 0.039528, -0.421448
H, -1.68476, -1.516905, -1.351806

$\left[\mathrm{Zn(OAc)(EtOH)_2}\right]^+(\mathrm{EtOH})$

Zn, 0.691655, 0.034431, 0.196146
O, 2.599933, -0.843201, 0.268643
O, 2.21878, 0.890325, -1.016115
O, -0.533536, 1.187335, 1.312633
O, -0.539333, -1.461604, -0.52709
C, 3.021616, 0.007671, -0.576281
C, 4.444296, -0.010815, -1.046533
H, 4.466133, 0.003597, -2.137063
H, 4.940132, 0.89531, -0.690903
H, 4.968443, -0.886255, -0.670221
C, -0.325127, -2.77172, 0.065025
C, -0.357583, -2.694214, 1.57642
H, -1.3347, -2.353358, 1.927959
H, -0.160635, -3.678938, 2.006807
H, 0.407992, -2.000629, 1.936581
H, -1.095276, -3.438619, -0.323104
H, 0.644982, -3.101507, -0.300596
H, -1.437985, -1.145118, -0.279234
C, -0.353494, 2.625923, 1.254144
C, -0.735755, 3.180009, -0.100041
H, -0.55182, 4.25699, -0.118534
H, -0.143393, 2.716487, -0.893076
H, -1.796115, 3.011842, -0.302172
H, -0.955565, 3.063907, 2.050163
H, 0.698808, 2.792356, 1.474987
H, -1.452776, 0.93515, 1.062047
O, -2.761504, -0.063663, 0.308397
C, -3.46509, 0.467195, -0.838865
H, -4.102771, 1.289287, -0.510759
H, -2.687831, 0.863525, -1.490582
C, -4.265363, -0.613216, -1.533572
H, -5.023737, -1.025015, -0.862856
H, -4.772786, -0.196251, -2.406718
H, -3.612535, -1.423476, -1.86655
H, -3.403935, -0.430741, 0.935902

$\left[\mathrm{Zn(OAc)(EtOH)_2}\right]^{+}\left(\mathrm{EtOH}\right)_2$

Zn, -1.447998, -0.125213, 0.081476
O, -2.894806, -1.683613, -0.282982
O, -3.454463, 0.278716, 0.515584
O, -0.566929, 1.017457, -1.370407
O, 0.137976, -0.689822, 1.226126
C, -3.790958, -0.890622, 0.136684
C, -5.232652, -1.299339, 0.154803
H, -5.73771, -0.868433, 1.018322
H, -5.707396, -0.906511, -0.748521
H, -5.325488, -2.383533, 0.156226
C, 0.592238, -2.05641, 1.03188
C, 0.91486, -2.329058, -0.421857
H, 1.689769, -1.649991, -0.785317
H, 1.275628, -3.354333, -0.535974
H, 0.023231, -2.20721, -1.043931
H, 1.462438, -2.2052, 1.672069
H, -0.218539, -2.687919, 1.389461
H, 0.849603, -0.069803, 0.924833
C, -1.265248, 2.23023, -1.756475
C, -1.337892, 3.209164, -0.605143
H, -1.916983, 4.087538, -0.899716
H, -1.825148, 2.749056, 0.259491
H, -0.338274, 3.540797, -0.314153
H, -0.739422, 2.655062, -2.611622
H, -2.254571, 1.906816, -2.074108
H, 0.311448, 1.248272, -0.98511
O, 1.712768, 1.231563, 0.15293
C, 2.002379, 2.201253, 1.18042
H, 2.425963, 3.094155, 0.716763
H, 1.039841, 2.461653, 1.619681
C, 2.938772, 1.626281, 2.224709
H, 3.907617, 1.379334, 1.784234
H, 3.102479, 2.356729, 3.020859
H, 2.512311, 0.722537, 2.668114
H, 2.54745, 0.93676, -0.281582
O, 3.862057, 0.097337, -1.06829
H, 4.511613, 0.568734, -1.610424
C, 4.542952, -0.863762, -0.240426
H, 5.344464, -0.365262, 0.308414
H, 3.798186, -1.208931, 0.477049
C, 5.080895, -2.016557, -1.063247
H, 5.572331, -2.74364, -0.411858
H, 4.270865, -2.519157, -1.596681
H, 5.813332, -1.661324, -1.792581

$\left[\mathrm{Zn(OAc)_2}\right]$

Zn, -0.000001, 0, -0.0037
O, 1.799527, 0.913437, 0.615009
O, -1.802727, 0.893171, -0.623718
C, 2.445991, 0.013331, -0.005944
C, -2.44599, -0.013332, -0.005935
O, 1.802725, -0.893172, -0.623723
O, -1.799523, -0.913437, 0.615014
C, 3.94403, -0.005849, 0.012584
C, -3.94403, 0.005849, 0.012583
H, 4.26377, -0.739404, 0.757609
H, 4.327571, -0.31968, -0.957552
H, 4.340604, 0.969914, 0.285278
H, -4.263782, 0.739623, 0.757385

H, -4.327554, 0.319407, -0.957649
H, -4.340607, -0.969839, 0.285539

$\left[\mathrm{Zn(OAc)_2(EtOH)}\right]$

Zn, 0.329854, -0.253127, -0.130427
O, -0.741824, 1.443597, -0.532787
O, -2.787612, -0.206666, -0.052522
O, 2.088169, -0.138064, 1.101804
O, 2.220864, -0.585589, -1.042284
O, -1.075338, -1.652275, -0.072664
C, 2.793442, -0.387616, 0.075276
C, -2.322894, -1.366414, 0.035213
C, -0.577707, 2.567719, 0.366434
H, 0.448551, 2.904718, 0.231454
H, -0.70316, 2.219526, 1.393547
C, -1.571422, 3.657651, 0.028491
H, -1.426356, 4.510896, 0.69548
H, -1.4376, 3.993455, -1.001907
H, -2.595373, 3.296252, 0.151778
H, -1.629815, 1.01869, -0.383172
C, 4.28743, -0.474735, 0.173857
H, 4.648079, 0.038499, 1.062966
H, 4.564001, -1.530612, 0.236517
H, 4.745376, -0.057196, -0.722348
C, -3.240738, -2.531783, 0.303047
H, -3.028916, -3.339567, -0.398781
H, -3.039042, -2.905651, 1.310242
H, -4.284102, -2.232145, 0.230767