Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
This journal is © The Owner Societies 2012

Additional Material for the manuscript "Investigation of Interstitial Hydrogen and related Defects in ZnO "

Jörg Koßmann and Christof Hättig

27th September 2012

Abstract

This document contains additional material to the above mentioned manuscript. In section 1 you can find the coordinates of the ideal (wurtzite) quantum cluster (without any defects or additional atoms, not relaxed), as well as the coordinates of the nearby point charges to which effective core potentials (ECPS) have been added. In section 2 the total electronic energies, Cartesian coordinates of all relaxed atoms after the geometry opitimizations, the zero point vibrational energies (ZPVE), unscaled vibrational frequencies and infra red (IR) intensities of all discussed structures are listed.

This journal is © The Owner Societies 2012

1 Quantum Cluster (without defects or additional atoms)

In this section the Cartesian coordinates of the ideal wurtzite quantum cluster (without any defect or additional atoms) which was used as starting point in our investigations are listed. Furthermore, you can find here the coordinates of the nearby pointcharges of the embedding to which effective core potentials (ECPs) have been added.

All coordinates of the quantum cluster in Å:

Zn	−1.62500000	0.93819420	−2.60382250	O	−1.62500000	0.93819420	−0.61182250
Zn	−1.62500000	0.93819420	2.60317750	O	−1.62500000	0.93819420	4.59517750
Zn	−3.25000000	3.75261160	−2.60382250	O	−1.62500000	2.81441740	−3.21500000
Zn	−1.62500000	6.56719420	−2.60382250	Zn	−1.62500000	2.81441740	0.00000000
O	−3.25000000	3.75261160	−0.61182250	Zn	−3.25000000	5.62900000	0.00000000
O	−1.68679320	6.60276480	−0.65137960	Zn	−3.25000000	3.75261160	2.60317750
O	−1.65869670	2.79404830	1.98247500	Zn	−1.62500000	6.56719420	2.60317750
O	−3.25000000	5.62900000	1.99200000	Zn	−1.62500000	2.81441740	5.20700000
O	−3.25000000	3.75261160	4.59517750	O	−1.62500000	6.56719420	4.59517750
Zn	−1.62500000	8.44341740	0.00000000	O	−1.62500000	8.44341740	1.99200000
O	1.62500000	0.93819420	−5.81882250	Zn	0.00000000	−1.87638840	−2.60382250
Zn	1.63090590	0.92522320	−2.58460250	O	0.00000000	0.00000000	−3.21500000
Zn	1.62500000	−2.81458260	0.00000000	O	0.00000000	−1.87638840	−0.61182250
Zn	0.00000000	0.00000000	0.00000000	O	1.64223220	0.93124300	−0.59623260
Zn	0.00000000	−1.87638840	2.60317750	O	1.62500000	−2.81458260	1.99200000
Zn	1.60527280	0.92388960	2.62505930	O	−0.03459570	−0.01891680	1.98246470
O	0.00000000	−1.87638840	4.59517750	Zn	0.00000000	0.00000000	5.20700000
O	1.61986740	0.94753040	4.62718230	Zn	1.62500000	0.93819420	7.81017750
Zn	1.62500000	2.81441740	−5.20700000	O	0.00000000	3.75261160	−5.81882250
Zn	0.00000000	5.62900000	−5.20700000	O	1.62500000	6.56719420	−5.81882250
Zn	−0.00815730	3.76389500	−2.58472900	O	1.61538400	2.80880180	−3.20096950
Zn	1.61095360	6.56835410	−2.58493030	O	−0.03762180	5.65044410	−3.23441590
Zn	1.62672200	2.81546690	0.02459290	O	0.00272800	3.77084720	−0.59640890
Zn	−0.04464070	5.65468290	0.00312180	O	1.61037510	6.55566790	−0.59665780
Zn	−0.02228590	3.74280540	2.62523740	O	1.61965630	2.81149090	2.02301070
Zn	1.62257180	6.59165400	2.62502320	O	0.00566000	5.62584650	1.99658410
Zn	1.61528240	2.80888280	5.27677730	O	0.00563790	3.74348910	4.62722470
Zn	0.00000000	5.62900000	5.20700000	O	1.63574190	6.56686920	4.62716720
Zn	0.00000000	3.75261160	7.81017750	O	1.60310520	2.80188710	7.29344610
Zn	1.62500000	6.56719420	7.81017750	O	0.00000000	5.62900000	7.19900000
Zn	0.00000000	9.38161160	−2.60382250	O	1.62500000	8.44341740	−3.21500000
Zn	1.62500000	8.44341740	0.00000000	O	0.00000000	9.38161160	−0.61182250
Zn	0.00000000	9.38161160	2.60317750	O	1.62588790	8.48307620	1.98233820
Zn	1.62500000	8.44341740	5.20700000	O	0.00000000	9.38161160	4.59517750
Zn	3.25000000	0.00000000	−5.20700000	O	4.87500000	0.93819420	−5.81882250
Zn	3.25000000	−1.87638840	−2.60382250	Zn	4.86907560	0.92518610	−2.58465400
O	3.24997170	−0.04330610	−3.23444670	Zn	4.87500000	−2.81458260	0.00000000
O	3.24998380	−1.94767800	−0.65140060	Zn	3.24999830	−0.05158510	0.00351210
O	4.85776050	0.93125050	−0.59629220	Zn	3.25000000	−1.87638840	2.60317750
O	4.87500000	−2.81458260	1.99200000	Zn	4.89495060	0.92394380	2.62504190
O	3.25013600	0.00640640	1.99684430	O	3.25000000	−1.87638840	4.59517750
Zn	3.25000000	0.00000000	5.20700000	O	4.88015400	0.94753130	4.62718300
Zn	4.87500000	0.93819420	7.81017750	O	3.25000000	0.00000000	7.19900000
Zn	4.87500000	2.81441740	−5.20700000	O	3.25000000	3.75261160	−5.81882250
Zn	3.25000000	5.62900000	−5.20700000	O	4.87500000	6.56719420	−5.81882250
Zn	3.24992050	3.75240910	−2.59741630	O	4.88453170	2.80877950	−3.20098340

Zn	4.88909350	6.56835970	−2.58492820	O	3.25002570	5.64006840	−3.20099350
Zn	4.87340770	2.81542960	0.02454350	O	3.24998270	3.75243720	−0.59964000
Zn	3.25006740	5.62699670	0.02367840	O	4.88971050	6.55571500	−0.59667090
Zn	3.25007690	3.75301300	2.66181740	O	4.88045650	2.81152670	2.02306600
Zn	4.87742040	6.59165550	2.62501730	O	3.24999900	5.63552980	2.02245040
Zn	4.88504600	2.80883280	5.27687580	O	3.25018000	3.75274280	4.66968220
Zn	3.25003340	5.64044620	5.27711440	O	4.86428200	6.56686840	4.62715490
Zn	3.25000000	3.75261160	7.81017750	O	4.89694080	2.80186620	7.29348320
Zn	4.87500000	6.56719420	7.81017750	O	3.24999530	5.65441550	7.29373440
Zn	3.25000000	9.38161160	−2.60382250	O	4.87500000	8.44341740	−3.21500000
Zn	4.87500000	8.44341740	0.00000000	O	3.25000000	9.38161160	−0.61182250
Zn	3.25000000	9.38161160	2.60317750	O	4.87411850	8.48307540	1.98234080
Zn	4.87500000	8.44341740	5.20700000	O	3.25000000	9.38161160	4.59517750
Zn	6.50000000	−1.87638840	−2.60382250	Zn	8.12500000	0.93819420	−2.60382250
O	6.50000000	0.00000000	−3.21500000	O	6.50000000	−1.87638840	−0.61182250
Zn	6.50000000	0.00000000	0.00000000	O	8.12500000	0.93819420	−0.61182250
Zn	6.50000000	−1.87638840	2.60317750	Zn	8.12500000	0.93819420	2.60317750
O	6.53470430	−0.01894900	1.98242130	O	6.50000000	−1.87638840	4.59517750
Zn	6.50000000	0.00000000	5.20700000	O	8.12500000	0.93819420	4.59517750
O	6.50000000	3.75261160	−5.81882250	Zn	6.50000000	5.62900000	−5.20700000
Zn	6.50811390	3.76388080	−2.58485180	O	8.12500000	2.81441740	−3.21500000
Zn	8.12500000	6.56719420	−2.60382250	O	6.53763410	5.65045790	−3.23444570
Zn	8.12500000	2.81441740	0.00000000	O	6.49737360	3.77094710	−0.59649880
Zn	6.54479100	5.65481620	0.00307360	O	8.18689910	6.60281680	−0.65142430
Zn	6.52232610	3.74288570	2.62510920	O	8.15870690	2.79407440	1.98247750
Zn	8.12500000	6.56719420	2.60317750	O	6.49432300	5.62592890	1.99653230
Zn	8.12500000	2.81441740	5.20700000	O	6.49450940	3.74356040	4.62715650
Zn	6.50000000	5.62900000	5.20700000	O	8.12500000	6.56719420	4.59517750
Zn	6.50000000	3.75261160	7.81017750	O	6.50000000	5.62900000	7.19900000
Zn	6.50000000	9.38161160	−2.60382250	Zn	8.12500000	8.44341740	0.00000000
O	6.50000000	9.38161160	−0.61182250	Zn	6.50000000	9.38161160	2.60317750
O	8.12500000	8.44341740	1.99200000	O	6.50000000	9.38161160	4.59517750
Zn	9.75000000	3.75261160	−2.60382250	O	9.75000000	3.75261160	−0.61182250
Zn	9.75000000	5.62900000	0.00000000	Zn	9.75000000	3.75261160	2.60317750
O	9.75000000	5.62900000	1.99200000	O	9.75000000	3.75261160	4.59517750

ECPs:

Zn	−8.12500000	2.81441740	0.00000000	Zn	−8.12500000	6.56719420	2.60317750
Zn	−8.12500000	2.81441740	5.20700000	Zn	−4.87500000	0.93819420	−2.60382250
Zn	−4.87500000	−2.81458260	0.00000000	Zn	−6.50000000	0.00000000	0.00000000
Zn	−4.87500000	0.93819420	2.60317750	Zn	−4.87500000	−2.81458260	5.20700000
Zn	−6.50000000	0.00000000	5.20700000	Zn	−4.87500000	0.93819420	7.81017750
Zn	−4.87500000	2.81441740	−5.20700000	Zn	−6.50000000	3.75261160	−2.60382250
Zn	−4.87500000	6.56719420	−2.60382250	Zn	−4.87500000	2.81441740	0.00000000
Zn	−6.50000000	5.62900000	0.00000000	Zn	−6.50000000	3.75261160	2.60317750
Zn	−4.87500000	6.56719420	2.60317750	Zn	−4.87500000	2.81441740	5.20700000
Zn	−6.50000000	5.62900000	5.20700000	Zn	−6.50000000	3.75261160	7.81017750
Zn	−4.87500000	6.56719420	7.81017750	Zn	−4.87500000	8.44341740	0.00000000
Zn	−6.50000000	9.38161160	2.60317750	Zn	−4.87500000	12.19619420	2.60317750
Zn	−4.87500000	8.44341740	5.20700000	Zn	−1.62500000	−4.69080580	−2.60382250
Zn	−3.25000000	−5.62900000	0.00000000	Zn	−1.62500000	−4.69080580	2.60317750
Zn	−3.25000000	−5.62900000	5.20700000	Zn	−1.62500000	−4.69080580	7.81017750
Zn	−1.62500000	0.93819420	−7.81082250	Zn	−1.62500000	−2.81458260	−5.20700000
Zn	−3.25000000	0.00000000	−5.20700000	Zn	−3.25000000	−1.87638840	−2.60382250
Zn	−1.62500000	−2.81458260	0.00000000	Zn	−3.25000000	0.00000000	0.00000000

Zn	−3.25000000	−1.87638840	2.60317750	Zn	−1.62500000	−2.81458260	5.20700000
Zn	−3.25000000	0.00000000	5.20700000	Zn	−3.25000000	−1.87638840	7.81017750
Zn	−1.62500000	0.93819420	7.81017750	Zn	−1.62500000	2.81441740	−10.41400000
Zn	−3.25000000	3.75261160	−7.81082250	Zn	−1.62500000	6.56719420	−7.81082250
Zn	−1.62500000	2.81441740	−5.20700000	Zn	−3.25000000	5.62900000	−5.20700000
Zn	−3.25000000	5.62900000	5.20700000	Zn	−3.25000000	3.75261160	7.81017750
Zn	−1.62500000	6.56719420	7.81017750	Zn	−1.62500000	2.81441740	10.41400000
Zn	−3.25000000	5.62900000	10.41400000	Zn	−1.62500000	8.44341740	−5.20700000
Zn	−3.25000000	9.38161160	−2.60382250	Zn	−1.62500000	12.19619420	−2.60382250
Zn	−3.25000000	11.25800000	0.00000000	Zn	−3.25000000	9.38161160	2.60317750
Zn	−1.62500000	12.19619420	2.60317750	Zn	−1.62500000	8.44341740	5.20700000
Zn	−3.25000000	11.25800000	5.20700000	Zn	−3.25000000	9.38161160	7.81017750
Zn	−1.62500000	12.19619420	7.81017750	Zn	−1.62500000	8.44341740	10.41400000
Zn	−1.62500000	14.07241740	0.00000000	Zn	−1.62500000	14.07241740	5.20700000
Zn	1.62500000	−4.69080580	−2.60382250	Zn	0.00000000	−5.62900000	0.00000000
Zn	0.00000000	−7.50538840	2.60317750	Zn	1.62500000	−4.69080580	2.60317750
Zn	0.00000000	−5.62900000	5.20700000	Zn	1.62500000	−4.69080580	7.81017750
Zn	0.00000000	0.00000000	−10.41400000	Zn	0.00000000	−1.87638840	−7.81082250
Zn	1.62500000	0.93819420	−7.81082250	Zn	1.62500000	−2.81458260	−5.20700000
Zn	0.00000000	0.00000000	−5.20700000	Zn	1.62500000	−2.81458260	5.20700000
Zn	0.00000000	−1.87638840	7.81017750	Zn	1.62500000	−2.81458260	10.41400000
Zn	0.00000000	0.00000000	10.41400000	Zn	1.62500000	2.81441740	−10.41400000
Zn	0.00000000	5.62900000	−10.41400000	Zn	0.00000000	3.75261160	−7.81082250
Zn	1.62500000	6.56719420	−7.81082250	Zn	1.62500000	2.81441740	10.41400000
Zn	0.00000000	5.62900000	10.41400000	Zn	1.62500000	8.44341740	−10.41400000
Zn	0.00000000	9.38161160	−7.81082250	Zn	1.62500000	8.44341740	−5.20700000
Zn	0.00000000	11.25800000	−5.20700000	Zn	1.62500000	12.19619420	−2.60382250
Zn	0.00000000	11.25800000	0.00000000	Zn	1.62500000	12.19619420	2.60317750
Zn	0.00000000	11.25800000	5.20700000	Zn	0.00000000	9.38161160	7.81017750
Zn	1.62500000	12.19619420	7.81017750	Zn	1.62500000	8.44341740	10.41400000
Zn	1.62500000	14.07241740	0.00000000	Zn	1.62500000	14.07241740	5.20700000
Zn	4.87500000	−4.69080580	−2.60382250	Zn	3.25000000	−5.62900000	0.00000000
Zn	3.25000000	−7.50538840	2.60317750	Zn	4.87500000	−4.69080580	2.60317750
Zn	3.25000000	−5.62900000	5.20700000	Zn	4.87500000	−4.69080580	7.81017750
Zn	3.25000000	0.00000000	−10.41400000	Zn	3.25000000	−1.87638840	−7.81082250
Zn	4.87500000	0.93819420	−7.81082250	Zn	4.87500000	−2.81458260	−5.20700000
Zn	4.87500000	−2.81458260	5.20700000	Zn	3.25000000	−1.87638840	7.81017750
Zn	4.87500000	−2.81458260	10.41400000	Zn	3.25000000	0.00000000	10.41400000
Zn	4.87500000	2.81441740	−10.41400000	Zn	3.25000000	5.62900000	−10.41400000
Zn	3.25000000	3.75261160	−7.81082250	Zn	4.87500000	6.56719420	−7.81082250
Zn	4.87500000	2.81441740	10.41400000	Zn	3.25000000	5.62900000	10.41400000
Zn	4.87500000	8.44341740	−10.41400000	Zn	3.25000000	9.38161160	−7.81082250
Zn	4.87500000	8.44341740	−5.20700000	Zn	3.25000000	11.25800000	−5.20700000
Zn	4.87500000	12.19619420	−2.60382250	Zn	3.25000000	11.25800000	0.00000000
Zn	4.87500000	12.19619420	2.60317750	Zn	3.25000000	11.25800000	5.20700000
Zn	3.25000000	9.38161160	7.81017750	Zn	4.87500000	12.19619420	7.81017750
Zn	4.87500000	8.44341740	10.41400000	Zn	4.87500000	14.07241740	0.00000000
Zn	4.87500000	14.07241740	5.20700000	Zn	8.12500000	−4.69080580	−2.60382250
Zn	6.50000000	−5.62900000	0.00000000	Zn	6.50000000	−7.50538840	2.60317750
Zn	8.12500000	−4.69080580	2.60317750	Zn	6.50000000	−5.62900000	5.20700000
Zn	8.12500000	−4.69080580	7.81017750	Zn	6.50000000	0.00000000	−10.41400000
Zn	6.50000000	−1.87638840	−7.81082250	Zn	8.12500000	0.93819420	−7.81082250
Zn	8.12500000	−2.81458260	−5.20700000	Zn	6.50000000	0.00000000	−5.20700000
Zn	8.12500000	−2.81458260	0.00000000	Zn	8.12500000	−2.81458260	5.20700000

Zn	6.50000000	−1.87638840	7.81017750	Zn	8.12500000	0.93819420	7.81017750
Zn	6.50000000	0.00000000	10.41400000	Zn	8.12500000	2.81441740	−10.41400000
Zn	6.50000000	5.62900000	−10.41400000	Zn	6.50000000	3.75261160	−7.81082250
Zn	8.12500000	6.56719420	−7.81082250	Zn	8.12500000	2.81441740	−5.20700000
Zn	8.12500000	6.56719420	7.81017750	Zn	8.12500000	2.81441740	10.41400000
Zn	6.50000000	5.62900000	10.41400000	Zn	6.50000000	9.38161160	−7.81082250
Zn	8.12500000	8.44341740	−5.20700000	Zn	6.50000000	11.25800000	−5.20700000
Zn	8.12500000	12.19619420	−2.60382250	Zn	6.50000000	11.25800000	0.00000000
Zn	8.12500000	12.19619420	2.60317750	Zn	8.12500000	8.44341740	5.20700000
Zn	6.50000000	11.25800000	5.20700000	Zn	6.50000000	9.38161160	7.81017750
Zn	8.12500000	12.19619420	7.81017750	Zn	8.12500000	8.44341740	10.41400000
Zn	8.12500000	14.07241740	0.00000000	Zn	8.12500000	14.07241740	5.20700000
Zn	9.75000000	−5.62900000	0.00000000	Zn	9.75000000	−5.62900000	5.20700000
Zn	9.75000000	0.00000000	−5.20700000	Zn	9.75000000	−1.87638840	−2.60382250
Zn	11.37500000	0.93819420	−2.60382250	Zn	11.37500000	−2.81458260	0.00000000
Zn	9.75000000	0.00000000	0.00000000	Zn	9.75000000	−1.87638840	2.60317750
Zn	11.37500000	0.93819420	2.60317750	Zn	11.37500000	−2.81458260	5.20700000
Zn	9.75000000	0.00000000	5.20700000	Zn	9.75000000	−1.87638840	7.81017750
Zn	11.37500000	0.93819420	7.81017750	Zn	9.75000000	3.75261160	−7.81082250
Zn	11.37500000	2.81441740	−5.20700000	Zn	9.75000000	5.62900000	−5.20700000
Zn	11.37500000	6.56719420	−2.60382250	Zn	11.37500000	2.81441740	0.00000000
Zn	11.37500000	6.56719420	2.60317750	Zn	11.37500000	2.81441740	5.20700000
Zn	9.75000000	5.62900000	5.20700000	Zn	9.75000000	3.75261160	7.81017750
Zn	11.37500000	6.56719420	7.81017750	Zn	9.75000000	5.62900000	10.41400000
Zn	9.75000000	9.38161160	−2.60382250	Zn	11.37500000	8.44341740	0.00000000
Zn	9.75000000	11.25800000	0.00000000	Zn	9.75000000	9.38161160	2.60317750
Zn	11.37500000	12.19619420	2.60317750	Zn	11.37500000	8.44341740	5.20700000
Zn	9.75000000	11.25800000	5.20700000	Zn	9.75000000	9.38161160	7.81017750
Zn	13.00000000	0.00000000	0.00000000	Zn	13.00000000	0.00000000	5.20700000
Zn	13.00000000	3.75261160	−2.60382250	Zn	14.62500000	2.81441740	0.00000000
Zn	13.00000000	5.62900000	0.00000000	Zn	13.00000000	3.75261160	2.60317750
Zn	14.62500000	6.56719420	2.60317750	Zn	14.62500000	2.81441740	5.20700000
Zn	13.00000000	5.62900000	5.20700000	Zn	13.00000000	3.75261160	7.81017750
Zn	13.00000000	9.38161160	2.60317750				

2 Detailed Results for all Species

In this section, the Cartesian coordinates of all relaxed atoms in the equilibrium structures of all species discussed in the manuscript are collected (Check the previous section for the coordinates of the fixed atoms and of the ECPs). Furthermore, also the total electronic energies, zero point vibrational energies (ZPVEs), unscaled vibrational frequencies, and infra red (IR) intensities are listed.

2.1 Interstitial Hydrogen

- $H_{AB_\perp}$

Energy (a.u.)	ZPVE (a.u.)
-154897.2676020	0.1632594

relaxed coordinates in Å:

H	2.72188900	2.29212370	1.62034260	O	−1.70285440	6.61185340	−0.65657300
O	−1.63120680	2.79382820	1.98409900	Zn	1.63295970	0.90720660	−2.60664960
O	1.64296590	0.92036180	−0.60382380	Zn	1.56092580	0.77360220	2.71647470
O	−0.06050920	−0.02984060	1.97564220	O	1.61437210	0.96333850	4.66629590
Zn	−0.02594570	3.78073290	−2.61576190	O	1.61222390	2.81065720	−3.17526420
Zn	1.61765960	6.58063710	−2.58755800	O	−0.04152530	5.66686970	−3.23791850
Zn	1.59531380	2.84279980	−0.22926510	O	−0.03579670	3.80863910	−0.60960220
Zn	−0.04990400	5.69154020	−0.00505260	O	1.61143140	6.55655160	−0.59851030
Zn	−0.06917060	3.79053550	2.64467580	O	1.86365820	2.69765970	1.92615830
Zn	1.62200190	6.62620800	2.64368690	O	0.03002490	5.61980900	1.99180070
Zn	1.62667620	2.81985000	5.32080050	O	0.02849310	3.72744080	4.60837650
O	1.63659680	6.56307170	4.64291330	O	1.59817130	2.80078550	7.32243460
O	1.62361190	8.49843690	1.97919260	Zn	4.88117690	0.92260040	−2.58102740
O	3.25846250	−0.05244440	−3.23517180	O	3.24872400	−1.95724220	−0.65451750
Zn	3.25647440	−0.06171650	−0.00453820	O	4.85359040	0.93536390	−0.58747500
Zn	4.90770340	0.92070940	2.64594990	O	3.24068450	0.02539680	1.99911190
O	4.87715270	0.95245930	4.64353610	Zn	3.27455600	3.76685150	−2.63468730
O	4.90083580	2.80288000	−3.19795990	Zn	4.89817480	6.57952420	−2.58396760
O	3.25516910	5.65596880	−3.20044340	Zn	4.88683150	2.82628520	0.00999750
O	3.26423130	3.76881840	−0.61845940	Zn	3.25897870	5.64346710	0.01545400
O	4.90186950	6.55788070	−0.59562070	Zn	3.40604220	3.93887140	2.80926130
O	4.84222350	2.81664070	2.02726060	Zn	4.91054180	6.63376300	2.63447210
O	3.25853840	5.70183120	2.01890630	Zn	4.90843280	2.79944850	5.31905380
O	3.26239020	3.77329200	4.75510510	Zn	3.25306460	5.68077040	5.33106000
O	4.86160560	6.56588390	4.63656680	O	4.89960540	2.79964260	7.32589000
O	3.24904680	5.65947420	7.33343810	O	4.87507840	8.50554870	1.97751880
O	6.53361660	−0.01826430	1.98340710	Zn	6.52175070	3.76610930	−2.58389470
O	6.54551220	5.65412590	−3.23542110	O	6.50367780	3.78004260	−0.59271080
Zn	6.55488530	5.66259930	0.00747410	O	8.19735560	6.60856770	−0.65577310
Zn	6.53365890	3.73785030	2.62593890	O	8.16048080	2.78928170	1.98129390
O	6.49012660	5.61996690	2.00166170	O	6.48899830	3.74003730	4.63002100

calculated wave numbers in cm^{-1} (unscaled):													
72	81	89	92	94	95	97	101	104	106	107	109	109	110
112	113	117	117	120	120	122	127	127	130	131	132	134	135
136	139	140	141	142	145	145	149	150	156	157	158	162	183
184	184	185	190	191	194	195	195	198	205	207	210	212	215
217	221	222	226	228	232	235	240	242	244	247	250	251	254
282	334	412	418	423	427	431	434	436	436	438	442	444	445
447	448	449	451	451	452	453	455	456	458	458	460	461	462
463	464	464	466	466	467	469	470	471	472	473	473	474	475
475	477	478	479	480	481	482	482	483	485	486	487	488	490
491	492	493	495	496	497	498	500	501	502	503	504	505	506
508	509	510	512	512	513	515	519	519	520	522	523	525	525
527	529	530	531	532	533	535	537	538	539	539	541	542	544
545	547	548	549	551	551	552	555	557	558	558	562	566	574
577	758	778	3306										

IR intensities in km/mol:													
1.9	2.8	0.0	0.0	0.1	0.1	0.5	0.4	0.7	0.2	0.4	0.0	0.1	0.1
0.1	0.1	0.1	0.0	0.1	0.1	0.2	0.2	0.3	0.0	0.7	1.2	0.0	0.5
0.0	0.2	0.3	0.1	0.1	0.3	0.6	0.5	0.7	0.2	0.2	0.1	0.6	1.5
1.3	0.3	0.4	0.0	0.2	0.1	0.1	0.2	0.0	1.1	1.9	0.9	0.6	0.4
0.3	0.3	2.9	2.3	0.6	1.4	1.7	2.7	4.6	0.8	3.5	7.7	4.3	7.7
21.1	26.2	61.3	29.8	31.4	21.4	25.3	1.6	7.7	54.0	6.5	28.1	24.6	178.4
35.9	9.6	10.8	38.5	13.5	23.0	59.0	241.0	118.2	2.2	75.9	35.5	119.9	50.0
5.2	31.1	9.4	8.6	35.5	8.7	13.5	16.1	45.0	75.3	60.8	17.7	93.8	31.8
41.6	19.1	43.2	86.2	32.0	81.4	31.7	97.2	235.1	22.4	39.5	14.4	3.8	1.4
107.9	43.0	13.7	43.1	5.6	34.8	74.1	84.5	57.8	38.4	102.5	25.0	36.8	6.3
94.0	27.4	20.0	24.4	18.8	5.3	45.8	15.0	29.5	26.7	43.2	21.5	54.5	63.4
28.2	26.9	41.9	47.0	38.7	31.3	22.9	25.2	12.7	13.2	1.9	25.6	11.5	27.8
19.3	7.2	24.1	6.2	18.0	3.0	5.6	9.8	5.7	7.3	3.9	1.4	5.7	24.7
32.4	5.7	2.4	47.6										

- $H_{AB_{\|}}$

Energy (a.u.)	ZPVE (a.u.)
-154897.2659227	0.1633404

relaxed coordinates in Å:

H	3.25063670	3.76549100	0.60768900	O	−1.69849100	6.60949660	−0.65902920
O	−1.65243980	2.79427650	1.97934280	Zn	1.62854680	0.90138310	−2.59885450
O	1.65458250	0.89904750	−0.61553820	Zn	1.60631790	0.92450420	2.64737250
O	−0.03111820	−0.01354130	1.97939460	O	1.61930420	0.95533630	4.64311890
Zn	−0.03013510	3.77370200	−2.59840260	O	1.61345470	2.80798330	−3.17016780
Zn	1.59068980	6.58236020	−2.60022890	O	−0.04788250	5.65580580	−3.24436900
Zn	1.45280980	2.71420970	0.03461610	O	−0.01853300	3.79716140	−0.61507950
Zn	−0.06869480	5.66809970	0.02838320	O	1.57491430	6.56207650	−0.61711040
Zn	−0.02152480	3.74273050	2.64790440	O	1.64244230	2.82486550	2.01391540
Zn	1.62338800	6.58977140	2.64689960	O	0.01230270	5.62171740	2.00756220
Zn	1.60264340	2.80162190	5.31912790	O	0.01193230	3.73905490	4.64344860
O	1.64290070	6.56350720	4.64252730	O	1.59979550	2.79998370	7.32670690
O	1.62896140	8.47707710	1.97924100	Zn	4.87185970	0.90160880	−2.59882690
O	3.25031920	−0.05447900	−3.24411230	O	3.25000400	−1.96128720	−0.65920460
Zn	3.25034090	−0.07903140	0.02783910	O	4.84577330	0.89933820	−0.61559960
Zn	4.89427950	0.92453870	2.64756480	O	3.25041970	0.01381050	2.00711640
O	4.88080460	0.95531430	4.64325440	Zn	3.25040710	3.75325840	−2.72091060
O	4.88722030	2.80803160	−3.17029010	Zn	4.90982160	6.58252640	−2.60021380
O	3.25037490	5.64352660	−3.17017200	Zn	5.04810430	2.71429790	0.03468930
O	3.25056320	3.75389850	−0.38788690	Zn	3.25051050	5.83578620	0.03018480
O	4.92591970	6.56225830	−0.61717870	Zn	3.25061730	3.75313930	2.78388670
O	4.85853420	2.82475380	2.01391380	Zn	4.87739220	6.58998960	2.64683210
O	3.25051270	5.60868090	2.00944360	Zn	4.89795440	2.80144410	5.31937330
O	3.25045770	3.75376660	4.75053620	Zn	3.25030020	5.65652290	5.32002390
O	4.85744010	6.56370330	4.64238420	O	4.90025490	2.79996520	7.32685920
O	3.25001500	5.65849140	7.32734390	O	4.87112890	8.47719960	1.97919060
O	6.53138290	−0.01367460	1.97932900	Zn	6.53050430	3.77394300	−2.59841510
O	6.54812810	5.65585800	−3.24449890	O	6.51904310	3.79750670	−0.61520620
Zn	6.56935640	5.66827260	0.02833940	O	8.19887440	6.60971010	−0.65916160
Zn	6.52221430	3.74277430	2.64800440	O	8.15273670	2.79412480	1.97925560
O	6.48812030	5.62153600	2.00741960	O	6.48832220	3.73914460	4.64345880

calculated wave numbers in cm^{-1} (unscaled):													
75	75	88	91	92	95	95	96	97	103	104	109	109	109
113	113	115	116	120	120	125	126	128	130	131	134	134	138
138	139	139	140	140	142	143	150	150	157	158	158	183	185
185	185	190	192	192	197	197	201	201	208	209	209	218	218
223	224	224	230	230	232	239	240	241	245	253	253	253	266
324	326	410	410	424	424	428	434	434	437	441	441	442	446
447	448	449	449	452	452	454	454	457	458	458	459	459	462
462	463	463	463	464	466	466	468	468	469	469	472	475	475
477	478	478	479	479	481	482	483	484	485	485	486	488	488
490	490	494	494	495	495	500	501	502	502	503	505	505	505
509	511	511	514	516	516	516	518	518	522	522	524	525	525
526	529	532	532	533	533	534	534	535	539	539	540	544	545
545	547	547	548	549	550	550	551	555	557	565	566	569	576
577	737	741	3317										

IR intensities in km/mol:													
0.9	0.9	0.0	0.1	0.2	0.0	0.2	0.0	2.9	0.0	0.1	0.2	0.1	0.0
0.1	0.1	0.3	0.0	0.1	0.0	0.1	0.1	0.0	1.4	0.0	0.0	0.0	0.0
0.2	0.0	0.7	0.3	0.3	0.1	0.0	0.6	0.7	0.0	0.0	0.1	0.1	1.8
1.8	0.1	0.1	0.1	0.1	0.0	0.0	0.0	2.1	0.5	0.8	1.1	0.1	0.1
0.5	0.0	0.0	2.0	0.4	0.6	0.0	0.6	0.7	10.2	14.1	12.8	3.0	2.9
21.8	21.6	0.0	0.1	39.1	38.7	212.4	18.1	19.0	0.0	0.2	1.7	1.9	39.4
33.0	0.7	8.0	6.9	3.0	2.5	355.7	0.1	49.0	55.3	104.2	76.7	71.8	0.0
196.3	0.2	0.4	0.5	100.1	48.0	49.1	35.8	77.2	45.7	43.3	0.1	121.6	121.8
43.9	0.3	0.9	12.7	12.0	80.2	62.9	4.2	6.6	175.9	147.8	1.8	26.4	25.4
17.5	12.2	31.4	16.0	25.2	45.8	83.9	12.2	0.3	24.4	25.0	49.9	42.0	47.5
0.3	56.0	57.9	134.7	0.2	2.8	3.4	52.3	51.6	33.3	36.0	3.5	1.9	1.9
26.6	0.1	9.8	10.6	0.3	0.1	1.9	1.2	0.3	96.7	98.0	7.4	0.5	40.9
42.5	6.7	9.2	11.8	0.2	0.6	0.7	0.0	36.0	9.5	20.9	20.2	4.1	43.3
43.7	1.4	1.5	62.4										

- $H_{BC_{\perp}}$

Energy (a.u.)	ZPVE (a.u.)
-154897.2686486	0.1635612

relaxed coordinates in Å:

O	−1.69430030	6.60712050	−0.65386130	O	−1.69070120	2.77719050	1.97314660
Zn	1.61634620	0.92434030	−2.58055630	O	1.64392590	0.93508570	−0.58896200
Zn	1.59499900	0.91116260	2.64152900	O	−0.03958520	−0.01971320	1.98319230
O	1.62072680	0.94946060	4.64257920	Zn	−0.02048640	3.76379940	−2.58031160
O	1.60333820	2.80622350	−3.19496590	Zn	1.60504300	6.57919430	−2.58038140
O	−0.04362580	5.65407360	−3.23230530	Zn	1.63277110	2.81928360	0.01821950
O	0.00540960	3.77322880	−0.58626030	Zn	−0.04987530	5.65783250	−0.00047790
O	1.60985620	6.55219070	−0.58643550	Zn	−0.10778970	3.73953120	2.62322970
O	1.58726290	2.80882290	2.03223630	Zn	1.58231000	6.66714360	2.62323710
O	0.01454090	5.62054770	2.00284820	Zn	1.56800130	2.76785490	5.36300090
O	0.01890060	3.73997120	4.62715470	O	1.64565040	6.55689230	4.62714960
O	1.59650880	2.79811390	7.35174030	O	1.62442400	8.51901520	1.97305240
Zn	4.86123230	0.89992720	−2.62724030	O	3.23165390	−0.05575060	−3.24073910
O	3.24952920	−1.96377190	−0.65719740	Zn	3.23586850	−0.06825630	−0.00421220
O	4.85151550	0.87595900	−0.63574280	Zn	4.89164180	0.83659270	2.64491500
O	3.23862330	0.01207030	1.99104460	O	4.87933670	0.96175770	4.62428650
Zn	3.23083090	3.76362860	−2.62096040	O	4.88641110	2.80796390	−3.17855000
Zn	4.88260340	6.58140170	−2.58067140	O	3.24628320	5.65171100	−3.19498480
Zn	4.93290790	2.78122230	−0.24556680	O	3.26612800	3.74328570	−0.59769980
Zn	3.24973590	5.61985900	0.01795360	O	4.88709420	6.55232350	−0.58916460
Zn	2.67351120	4.08602620	2.98727040	O	5.03903500	2.71857210	1.86054250
H	4.18680500	3.20691570	1.89964220	Zn	4.88301690	6.60655650	2.64166910
O	3.23568400	5.66490700	2.03180670	Zn	4.88263210	2.81005100	5.29812560
O	3.21224090	3.77444870	4.81333870	Zn	3.26187630	5.70161530	5.36345160
O	4.86282570	6.56501790	4.64265950	O	4.90016430	2.80000770	7.30943370
O	3.25000090	5.66209220	7.35216670	O	4.87227730	8.48747920	1.98317260
O	6.54503960	−0.02312650	1.97883910	Zn	6.52624190	3.78366580	−2.62701080
O	6.53918250	5.67269550	−3.24075090	O	6.54212160	3.80436300	−0.63544340
Zn	6.55188900	5.67556330	−0.00392590	O	8.20041540	6.61123540	−0.65703220
Zn	6.59480660	3.78868730	2.64475190	O	8.16695360	2.78723570	1.97905970
O	6.48344050	5.63267650	1.99138220	O	6.48155920	3.73697040	4.62420070

calculated wave numbers in cm^{-1} (unscaled):													
64	69	86	92	93	95	96	99	104	107	107	108	109	110
112	114	116	116	118	120	121	126	128	128	129	131	133	134
136	139	139	141	144	145	145	148	150	155	157	158	165	183
184	184	188	190	192	193	194	197	198	205	209	210	213	217
220	223	224	229	233	236	239	240	244	247	249	250	253	289
353	372	398	399	419	423	426	427	430	436	438	438	442	444
445	447	448	449	452	454	454	456	456	458	458	459	461	462
463	463	464	465	466	467	468	470	470	471	472	472	474	475
477	478	479	479	481	481	483	483	485	486	487	489	490	490
492	492	495	496	498	499	499	500	501	501	504	505	506	506
507	510	512	512	512	515	518	519	520	520	522	525	525	526
526	528	529	529	531	535	536	538	539	540	540	541	542	543
546	547	550	550	551	553	554	555	558	562	563	566	571	576
579	584	702	3534										

IR intensities in km/mol:													
0.2	1.3	0.1	0.0	0.0	0.0	0.8	0.1	0.1	0.1	0.2	0.0	0.0	0.0
0.0	0.0	0.1	0.1	0.0	0.1	0.0	0.8	0.0	0.4	0.2	0.0	0.2	0.8
0.0	0.2	0.2	0.3	0.4	0.3	0.1	0.7	0.7	0.1	0.3	0.2	0.4	0.2
1.1	1.7	0.5	0.1	0.1	0.1	0.3	0.1	0.0	1.7	1.5	0.7	0.1	0.0
1.6	0.9	0.5	1.4	0.5	3.3	3.3	3.5	0.2	1.1	4.6	10.9	9.4	8.1
4.9	45.2	23.0	50.7	52.9	0.6	33.4	9.5	26.2	4.3	0.0	2.3	1.0	6.4
254.5	81.4	6.8	106.0	3.0	5.1	216.5	105.7	70.4	8.1	40.5	49.8	2.5	12.8
12.7	12.9	9.5	24.1	10.5	29.8	47.4	1.9	3.0	1.6	139.4	38.7	112.8	20.3
4.0	48.1	15.9	35.2	34.9	109.3	261.6	69.2	20.9	42.4	44.2	9.0	53.0	16.6
43.7	1.8	132.9	2.8	55.0	85.2	14.8	33.2	124.5	258.4	24.3	61.7	55.3	41.6
2.3	46.1	8.2	1.6	9.9	25.2	15.3	19.6	47.5	17.1	53.8	0.7	54.7	57.6
8.9	12.0	14.7	173.3	76.3	64.2	10.8	19.7	0.8	36.5	20.0	50.2	8.6	15.5
0.6	0.8	8.1	10.5	4.0	1.3	5.7	15.2	2.5	9.9	5.5	4.1	1.9	27.9
0.6	27.9	0.5	100.0										

- $H_{BC_{\parallel}}$

Energy (a.u.)	ZPVE (a.u.)
-154897.2715143	0.1636746

relaxed coordinates in Å:

H	1.87142960	2.96534460	1.24452450	O	−1.69522040	6.60605630	−0.65797060
O	−1.65205360	2.79259470	1.97886940	Zn	1.65745880	0.83320550	−2.65376770
O	1.65343650	0.87888380	−0.63419910	Zn	1.61343510	0.84908260	2.66828660
O	−0.03216680	−0.01221450	1.97876500	O	1.61676730	0.96028360	4.64637070
Zn	−0.07428800	3.83267870	−2.65294950	O	1.62626310	2.81496060	−3.10228170
Zn	1.62682690	6.59354310	−2.56853050	O	−0.03296140	5.69651120	−3.25052720
Zn	1.60426890	2.80102080	−0.80325320	O	−0.03559340	3.80567850	−0.63304420
Zn	−0.04556020	5.68073180	0.01620660	O	1.61438840	6.54883270	−0.58789610
Zn	−0.08505630	3.78805430	2.67016230	O	1.67936020	2.84798270	2.20220610
Zn	1.62707920	6.60769660	2.64641760	O	0.01690020	5.62858950	2.00044320
Zn	1.61817010	2.81034750	5.32186210	O	0.01486900	3.73438730	4.64762430
O	1.63890500	6.56332260	4.64563420	O	1.59893410	2.79945730	7.32707310
O	1.62559970	8.48777750	1.98061050	Zn	4.89885610	0.92635690	−2.56851820
O	3.29244320	−0.06264780	−3.25076630	O	3.24864690	−1.95732340	−0.65827270
Zn	3.27217530	−0.06631220	0.01622830	O	4.85371410	0.93764630	−0.58784350
Zn	4.91112220	0.91921320	2.64629810	O	3.25797330	0.01456870	2.00027440
O	4.87872190	0.95183100	4.64556480	Zn	3.35297890	3.81211470	−2.65738040
O	4.92347790	2.79924940	−3.20575400	Zn	4.91053000	6.59069140	−2.56821380
O	3.26133360	5.67858250	−3.20575500	Zn	4.88200300	2.81286610	0.05257380
O	3.26649550	3.76182800	−0.60559850	Zn	3.25265480	5.63549800	0.05230420
O	4.89094750	6.55001260	−0.58439170	Zn	3.40366230	3.84096990	2.81369680
O	4.89300300	2.81212420	2.04734310	Zn	4.89581910	6.61651130	2.63909770
O	3.25709670	5.64520930	2.04728170	Zn	4.91191700	2.79624210	5.32628430
O	3.26556410	3.76143730	4.77634950	Zn	3.25275170	5.66986200	5.32650100
O	4.86085260	6.56600760	4.64106880	O	4.90099900	2.79886230	7.33250900
O	3.24944310	5.65948650	7.33280730	O	4.87359450	8.49480130	1.97944060
O	6.53887300	−0.02171240	1.98073710	Zn	6.53812700	3.77157660	−2.56851690
O	6.54369890	5.65425940	−3.23501460	O	6.49292970	3.77451240	−0.58454060
Zn	6.55148210	5.65815300	0.01621590	O	8.19265960	6.60613710	−0.65567190
Zn	6.55345380	3.74560110	2.63929410	O	8.16906440	2.78748800	1.97938410
O	6.49133690	5.62358880	2.00652630	O	6.49205830	3.74095590	4.64114400

calculated wave numbers in cm^{-1} (unscaled):													
60	76	91	92	95	95	97	98	105	106	107	109	109	111
112	112	114	116	118	121	122	129	129	131	131	133	134	135
137	139	141	141	142	146	147	152	154	157	158	159	163	182
185	185	186	192	193	197	197	198	200	206	209	210	216	221
223	224	226	230	236	240	241	242	249	250	251	255	258	315
359	372	376	382	390	405	425	432	437	438	440	443	444	446
449	450	450	451	452	453	454	456	457	458	458	459	460	461
463	464	465	465	466	468	468	468	469	470	470	472	473	475
476	478	479	480	481	481	482	483	483	485	485	487	488	488
491	492	492	493	496	497	498	500	502	504	504	506	507	509
509	511	511	512	515	516	516	518	520	521	523	523	525	525
527	527	529	531	532	534	534	534	536	536	539	544	544	547
547	548	548	550	552	553	555	556	556	557	575	578	579	579
582	598	676	3524										

IR intensities in km/mol:													
0.5	0.2	0.1	0.1	0.0	0.0	0.1	0.0	0.2	0.4	0.1	0.0	0.3	0.0
0.0	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.2	0.1	0.1	0.0	0.1	0.0
1.4	0.1	0.2	0.2	0.0	0.3	0.0	0.5	0.4	0.1	0.3	0.2	0.4	0.2
0.6	1.1	0.4	0.1	0.1	0.1	0.4	0.6	0.0	0.4	0.6	0.2	0.0	0.1
0.2	1.1	1.9	0.8	0.3	4.7	0.4	3.1	3.5	0.0	5.8	12.4	11.8	5.6
29.7	9.4	49.3	25.9	6.7	36.1	9.9	85.5	11.3	6.7	1.9	42.5	4.2	180.0
2.9	184.0	23.6	28.9	7.2	81.7	7.2	73.4	46.9	52.7	20.6	16.4	4.4	2.8
136.3	12.4	60.0	24.9	92.8	65.7	39.9	17.1	32.5	3.7	135.8	27.0	45.8	4.0
104.9	30.1	17.8	150.2	3.6	39.7	23.0	5.3	63.8	123.5	122.6	19.8	1.4	0.0
18.5	0.7	15.7	73.2	1.9	37.9	1.7	127.3	37.1	99.8	79.8	26.0	17.8	3.0
30.8	41.9	28.2	19.5	29.8	48.8	26.8	36.5	14.2	46.3	88.6	12.3	14.9	13.9
12.9	2.7	31.0	2.4	30.4	8.5	7.5	4.3	20.2	154.6	24.9	8.1	34.1	19.3
9.1	1.9	14.5	18.0	17.1	0.3	12.8	2.2	13.3	7.8	8.8	38.9	25.5	29.7
6.9	0.8	0.4	82.4										

- $H_{BC_{\parallel}}$

Energy (a.u.)	ZPVE (a.u.)
-154897.2715143	0.1636746

relaxed coordinates in Å:

H	1.87142960	2.96534460	1.24452450	O	−1.69522040	6.60605630	−0.65797060
O	−1.65205360	2.79259470	1.97886940	Zn	1.65745880	0.83320550	−2.65376770
O	1.65343650	0.87888380	−0.63419910	Zn	1.61343510	0.84908260	2.66828660
O	−0.03216680	−0.01221450	1.97876500	O	1.61676730	0.96028360	4.64637070
Zn	−0.07428800	3.83267870	−2.65294950	O	1.62626310	2.81496060	−3.10228170
Zn	1.62682690	6.59354310	−2.56853050	O	−0.03296140	5.69651120	−3.25052720
Zn	1.60426890	2.80102080	−0.80325320	O	−0.03559340	3.80567850	−0.63304420
Zn	−0.04556020	5.68073180	0.01620660	O	1.61438840	6.54883270	−0.58789610
Zn	−0.08505630	3.78805430	2.67016230	O	1.67936020	2.84798270	2.20220610
Zn	1.62707920	6.60769660	2.64641760	O	0.01690020	5.62858950	2.00044320
Zn	1.61817010	2.81034750	5.32186210	O	0.01486900	3.73438730	4.64762430
O	1.63890500	6.56332260	4.64563420	O	1.59893410	2.79945730	7.32707310
O	1.62559970	8.48777750	1.98061050	Zn	4.89885610	0.92635690	−2.56851820
O	3.29244320	−0.06264780	−3.25076630	O	3.24864690	−1.95732340	−0.65827270
Zn	3.27217530	−0.06631220	0.01622830	O	4.85371410	0.93764630	−0.58784350
Zn	4.91112220	0.91921320	2.64629810	O	3.25797330	0.01456870	2.00027440
O	4.87872190	0.95183100	4.64556480	Zn	3.35297890	3.81211470	−2.65738040
O	4.92347790	2.79924940	−3.20575400	Zn	4.91053000	6.59069140	−2.56821380
O	3.26133360	5.67858250	−3.20575500	Zn	4.88200300	2.81286610	0.05257380
O	3.26649550	3.76182800	−0.60559850	Zn	3.25265480	5.63549800	0.05230420
O	4.89094750	6.55001260	−0.58439170	Zn	3.40366230	3.84096990	2.81369680
O	4.89300300	2.81212420	2.04734310	Zn	4.89581910	6.61651130	2.63909770
O	3.25709670	5.64520930	2.04728170	Zn	4.91191700	2.79624210	5.32628430
O	3.26556410	3.76143730	4.77634950	Zn	3.25275170	5.66986200	5.32650100
O	4.86085260	6.56600760	4.64106880	O	4.90099900	2.79886230	7.33250900
O	3.24944310	5.65948650	7.33280730	O	4.87359450	8.49480130	1.97944060
O	6.53887300	−0.02171240	1.98073710	Zn	6.53812700	3.77157660	−2.56851690
O	6.54369890	5.65425940	−3.23501460	O	6.49292970	3.77451240	−0.58454060
Zn	6.55148210	5.65815300	0.01621590	O	8.19265960	6.60613710	−0.65567190
Zn	6.55345380	3.74560110	2.63929410	O	8.16906440	2.78748800	1.97938410
O	6.49133690	5.62358880	2.00652630	O	6.49205830	3.74095590	4.64114400

calculated wave numbers in cm^{-1} (unscaled):													
60	76	91	92	95	95	97	98	105	106	107	109	109	111
112	112	114	116	118	121	122	129	129	131	131	133	134	135
137	139	141	141	142	146	147	152	154	157	158	159	163	182
185	185	186	192	193	197	197	198	200	206	209	210	216	221
223	224	226	230	236	240	241	242	249	250	251	255	258	315
359	372	376	382	390	405	425	432	437	438	440	443	444	446
449	450	450	451	452	453	454	456	457	458	458	459	460	461
463	464	465	465	466	468	468	468	469	470	470	472	473	475
476	478	479	480	481	481	482	483	483	485	485	487	488	488
491	492	492	493	496	497	498	500	502	504	504	506	507	509
509	511	511	512	515	516	516	518	520	521	523	523	525	525
527	527	529	531	532	534	534	534	536	536	539	544	544	547
547	548	548	550	552	553	555	556	556	557	575	578	579	579
582	598	676	3524										

IR intensities in km/mol:													
0.5	0.2	0.1	0.1	0.0	0.0	0.1	0.0	0.2	0.4	0.1	0.0	0.3	0.0
0.0	0.1	0.1	0.0	0.1	0.0	0.0	0.1	0.2	0.1	0.1	0.0	0.1	0.0
1.4	0.1	0.2	0.2	0.0	0.3	0.0	0.5	0.4	0.1	0.3	0.2	0.4	0.2
0.6	1.1	0.4	0.1	0.1	0.1	0.4	0.6	0.0	0.4	0.6	0.2	0.0	0.1
0.2	1.1	1.9	0.8	0.3	4.7	0.4	3.1	3.5	0.0	5.8	12.4	11.8	5.6
29.7	9.4	49.3	25.9	6.7	36.1	9.9	85.5	11.3	6.7	1.9	42.5	4.2	180.0
2.9	184.0	23.6	28.9	7.2	81.7	7.2	73.4	46.9	52.7	20.6	16.4	4.4	2.8
136.3	12.4	60.0	24.9	92.8	65.7	39.9	17.1	32.5	3.7	135.8	27.0	45.8	4.0
104.9	30.1	17.8	150.2	3.6	39.7	23.0	5.3	63.8	123.5	122.6	19.8	1.4	0.0
18.5	0.7	15.7	73.2	1.9	37.9	1.7	127.3	37.1	99.8	79.8	26.0	17.8	3.0
30.8	41.9	28.2	19.5	29.8	48.8	26.8	36.5	14.2	46.3	88.6	12.3	14.9	13.9
12.9	2.7	31.0	2.4	30.4	8.5	7.5	4.3	20.2	154.6	24.9	8.1	34.1	19.3
9.1	1.9	14.5	18.0	17.1	0.3	12.8	2.2	13.3	7.8	8.8	38.9	25.5	29.7
6.9	0.8	0.4	82.4										

- H_{cage}

Energy (a.u.)	ZPVE (a.u.)
-154897.2322884	0.1582086

relaxed coordinates in Å:

H	1.67310450	4.65964740	0.81659320	O	−1.67896850	6.59824310	−0.64805450
O	−1.65645000	2.79395020	1.98371760	Zn	1.62154480	0.92599660	−2.57082730
O	1.63962250	0.95798000	−0.57727910	Zn	1.60381790	0.88589300	2.64529970
O	−0.04262420	−0.02576300	1.98159540	O	1.61935240	0.94676060	4.64646780
Zn	−0.01198950	3.76056770	−2.60266630	O	1.61275210	2.80371320	−3.20084560
Zn	1.61210050	6.57348590	−2.60245120	O	−0.04522800	5.65502070	−3.23797650
Zn	1.64146660	2.85220450	0.04020720	O	−0.01788220	3.75848240	−0.62273470
Zn	−0.02433260	5.64284820	0.00666230	O	1.61080740	6.57936670	−0.62246580
Zn	−0.01662290	3.73688450	2.63840770	O	1.62461200	2.77236150	2.06797830
Zn	1.63038340	6.58918400	2.63830440	O	−0.00037840	5.62910100	2.02040780
Zn	1.61541570	2.80698880	5.28955470	O	0.00908160	3.74069750	4.64226530
O	1.63991830	6.56519920	4.64218800	O	1.60133370	2.80062550	7.30965960
O	1.62706280	8.48081810	1.98373360	Zn	4.87330180	0.91936840	−2.58337610
O	3.24426020	−0.04764090	−3.22935580	O	3.24840140	−1.94993330	−0.65310040
Zn	3.24202010	−0.04619450	0.00587150	O	4.85690800	0.92014340	−0.59369880
Zn	4.89647570	0.91987400	2.63369020	O	3.25467410	0.00351260	1.99936570
O	4.88053440	0.95030500	4.63814050	Zn	3.25927160	3.74724160	−2.63304030
O	4.90181070	2.79896860	−3.20280690	Zn	4.88360880	6.57607670	−2.57073570
O	3.25306000	5.64480800	−3.20091110	Zn	4.90023120	2.79984160	0.03072830
O	3.30147240	3.72275250	−0.64304960	Zn	3.22510320	5.59550750	0.04050080
O	4.86474880	6.54452120	−0.57729260	Zn	3.25155350	3.75180120	2.68182400
O	4.88205980	2.81021930	2.03187740	Zn	4.90954670	6.61159690	2.64544020
O	3.28630870	5.65028240	2.06803550	Zn	4.88817290	2.80692210	5.29085090
O	3.25238940	3.75122780	4.69522620	Zn	3.25165770	5.64101510	5.28969560
O	4.86463500	6.56766840	4.64659210	O	4.89934580	2.80047260	7.30989340
O	3.25019560	5.65652410	7.30988410	O	4.87600220	8.49318750	1.98157750
O	6.53788020	−0.01971810	1.98262470	Zn	6.51536590	3.76353080	−2.58335270
O	6.53837370	5.65780670	−3.22935770	O	6.50646130	3.77723890	−0.59361340
Zn	6.53559890	5.65900510	0.00591600	O	8.18776100	6.60521190	−0.65294370
Zn	6.52643650	3.74306220	2.63364600	O	8.16096860	2.79155620	1.98261530
O	6.49917240	5.62305130	1.99951400	O	6.49222250	3.74175000	4.63807730

calculated wave numbers in cm^{-1} (unscaled):													
89	94	95	96	98	98	109	109	110	111	111	112	113	113
114	116	120	121	122	123	128	130	131	131	133	135	136	137
141	142	143	144	145	145	147	152	153	155	158	159	183	183
184	186	190	191	193	196	198	198	207	208	209	211	215	219
222	224	228	229	232	234	240	241	242	245	248	251	253	404
410	418	424	427	432	432	437	438	438	438	440	441	442	447
448	448	449	449	451	451	452	454	454	455	456	458	459	460
461	462	464	464	465	466	466	466	467	469	471	471	472	473
473	474	476	478	480	480	481	481	483	484	484	485	486	488
489	489	491	492	494	496	497	500	502	502	503	504	506	507
510	513	513	514	514	517	518	521	522	523	524	524	525	526
526	529	531	531	533	534	535	535	539	540	540	541	542	543
544	545	547	548	548	550	550	551	553	555	555	558	561	574
574	637	673	727										

IR intensities in km/mol:													
0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.1	0.0
0.1	0.0	0.0	0.1	0.2	0.0	0.0	0.4	0.5	0.0	0.1	0.0	0.0	0.0
0.2	0.3	0.4	0.1	0.4	0.5	0.1	1.1	0.9	0.0	0.1	0.1	2.0	2.1
0.0	0.1	0.3	0.1	0.0	0.1	0.2	0.0	3.1	1.4	3.5	0.3	0.6	1.4
0.8	1.7	0.6	1.0	3.0	4.1	3.2	0.3	0.3	1.1	4.7	8.2	10.3	5.2
65.5	6.9	25.2	158.2	8.1	3.0	16.6	23.9	4.1	14.5	14.9	11.3	76.6	239.0
14.2	3.9	65.9	69.7	43.5	9.8	25.8	103.5	69.7	43.6	25.7	65.2	175.5	108.2
169.2	196.4	19.5	18.4	17.0	108.6	15.8	17.2	88.7	234.1	54.0	17.3	7.3	0.7
35.7	33.4	18.9	11.0	103.0	56.2	93.8	18.1	67.9	9.4	147.8	12.7	111.1	129.7
6.4	59.0	142.2	1.9	31.7	101.4	116.0	23.6	32.1	21.7	278.9	123.8	207.7	1.0
169.7	36.9	212.2	184.1	364.3	176.3	129.8	3.5	22.1	96.2	137.9	13.0	300.1	413.8
47.4	44.8	116.7	85.8	10.2	60.5	155.2	35.1	33.6	13.2	40.5	30.2	158.5	19.6
101.4	0.4	74.4	36.4	36.6	25.5	13.5	15.5	43.7	20.0	36.4	17.8	13.4	137.8
135.8	169.4	189.5	167.4										

- $(H_2)_{cage}$

Energy (a.u.)	ZPVE (a.u.)
-154897.8423839	0.1716443

relaxed coordinates in Å:

H	1.68372130	4.64673450	1.19819380	H	1.60935600	4.70518230	0.44056200
O	−1.70621210	6.61406460	−0.66000370	O	−1.65845630	2.79259520	1.98394250
Zn	1.62891220	0.91787960	−2.59653840	O	1.65210160	0.89928100	−0.60556170
Zn	1.60541000	0.88218460	2.65573610	O	−0.04144270	−0.02510770	1.98100300
O	1.61948760	0.94528870	4.65460230	Zn	−0.01242560	3.75904410	−2.58709260
O	1.61297620	2.80288780	−3.19740150	Zn	1.61338810	6.57472100	−2.58666280
O	−0.04394460	5.65456890	−3.23270870	Zn	1.64416030	2.75819640	0.01672730
O	−0.00672270	3.76054110	−0.60595350	Zn	−0.08148270	5.67545030	−0.00243510
O	1.61524990	6.56826500	−0.60532330	Zn	−0.01937200	3.73162710	2.63743220
O	1.62771550	2.75568230	2.06124940	Zn	1.63336860	6.59342340	2.63631120
O	−0.01442830	5.63664920	2.02148740	Zn	1.61534530	2.80696130	5.28964480
O	0.00996050	3.74022660	4.64026560	O	1.64067480	6.56467730	4.63963310
O	1.60145620	2.80105510	7.30952100	O	1.62723150	8.48307260	1.98389120
Zn	4.87591350	0.92176370	−2.58413900	O	3.25418760	−0.05229290	−3.23467470
O	3.25055240	−1.96167520	−0.65622190	Zn	3.26104570	−0.06774620	0.00994290
O	4.85747950	0.92179260	−0.59411510	Zn	4.89865820	0.91903000	2.63329560
O	3.25675830	0.00205280	2.00007330	O	4.88051360	0.95057160	4.63765070
Zn	3.25691650	3.74861770	−2.61381670	O	4.89788360	2.80116300	−3.20138130
Zn	4.89461520	6.57366910	−2.59684450	O	3.25400870	5.64514080	−3.19737330
Zn	4.88808750	2.80665650	0.02217230	O	3.28093410	3.73540910	−0.62346740
Zn	3.31035130	5.64117210	0.01735580	O	4.92340030	6.56348950	−0.60604640
Zn	3.26348360	3.74500530	2.68274360	O	4.88763780	2.80696270	2.02767170
Zn	4.91319380	6.61179500	2.65558390	O	3.30219730	5.65567210	2.06051590
Zn	4.88871530	2.80663570	5.29122950	O	3.25244250	3.75135720	4.69325670
Zn	3.25143490	5.64139190	5.28991930	O	4.86590560	6.56822720	4.65448890
O	4.89925350	2.80053700	7.30949180	O	3.24988290	5.65623350	7.30987420
O	4.87593540	8.49176160	1.98098480	O	6.53905860	−0.02074320	1.98218630
Zn	6.51454840	3.75964740	−2.58398850	O	6.54756800	5.65117440	−3.23462200
O	6.50529020	3.77556070	−0.59403240	Zn	6.56477010	5.65283240	0.00984760
O	8.19941610	6.60936620	−0.65617050	Zn	6.52819430	3.74164270	2.63323280
O	8.16238560	2.79111320	1.98220960	O	6.50150740	5.62190530	2.00003220
O	6.49197170	3.74162200	4.63752750				

calculated wave numbers in cm^{-1} (unscaled):													
89	93	94	95	97	98	105	108	109	109	111	111	112	113
115	117	120	121	123	125	130	130	131	132	135	135	136	141
142	142	144	145	145	146	150	152	155	158	159	164	182	184
185	187	189	191	193	196	198	199	206	209	209	211	215	218
221	225	229	229	230	231	237	239	242	245	250	250	252	401
405	415	423	424	425	429	432	435	437	437	439	442	444	445
445	446	448	449	451	451	452	453	453	456	456	457	458	459
461	463	464	465	465	467	467	467	469	470	470	471	472	473
475	475	478	479	480	481	482	482	483	484	486	487	488	489
490	490	493	494	496	498	498	501	502	503	504	505	507	509
510	512	515	515	515	517	518	519	522	523	523	525	526	527
528	529	533	534	534	534	536	536	541	542	542	542	544	544
545	545	545	546	548	549	550	553	555	558	559	562	562	564
573	575	576	696	949	968	4134							

IR intensities in km/mol:													
0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0
0.0	0.0	0.2	0.3	0.1	0.0	0.2	0.3	0.5	0.1	0.0	0.1	0.1	0.0
0.3	0.5	0.3	0.2	0.2	0.5	0.4	1.2	0.2	0.0	0.1	0.6	1.5	2.4
0.5	0.0	0.0	0.3	0.1	0.1	0.0	0.0	2.3	2.7	1.2	1.2	0.0	2.9
0.3	0.6	0.7	0.7	0.3	0.8	4.7	1.1	2.5	1.8	12.4	4.1	7.1	0.4
111.8	17.7	30.5	94.8	1.2	23.9	45.0	3.3	6.2	19.5	1.3	105.3	0.8	18.5
66.8	43.8	86.9	21.0	42.1	17.3	10.5	112.0	45.2	77.1	44.0	0.2	71.1	5.3
693.4	21.1	30.8	4.9	0.7	176.1	20.2	1.5	58.5	264.9	158.8	4.0	11.4	16.8
12.1	12.1	8.7	11.1	70.1	4.8	63.3	106.7	16.0	94.6	81.0	174.8	46.6	91.9
119.3	38.8	3.0	71.3	52.5	166.7	44.5	96.7	95.1	106.3	21.4	47.4	219.4	160.8
147.4	123.3	2.8	278.2	300.4	203.2	25.2	139.9	99.3	42.8	16.6	129.9	295.5	119.3
7.6	34.5	299.7	71.9	15.7	40.0	106.8	58.0	301.0	179.1	58.4	1.1	25.1	69.8
58.9	25.4	11.6	164.0	74.8	73.2	33.5	33.9	31.6	12.4	28.6	4.2	38.0	39.5
54.9	203.4	160.0	22.8	5.8	4.2	0.4							

- $2H_{BC_{\perp}}$

Energy (a.u.)	ZPVE (a.u.)
-154897.8307275	0.1727246

relaxed coordinates in Å:

O	−1.69378090	6.60915990	−0.65525490	O	−1.71621910	2.77321710	1.96671680
Zn	1.61789670	0.92380580	−2.58348290	O	1.64315210	0.93354400	−0.59949300
Zn	1.62643740	0.96385960	2.62558210	O	−0.02659980	−0.01424080	1.98696800
O	1.61586570	0.95452240	4.64270740	Zn	−0.02076670	3.76744010	−2.59373960
O	1.60399950	2.80784650	−3.19895690	Zn	1.61038510	6.57879600	−2.57118960
O	−0.03918400	5.66304480	−3.23346840	Zn	1.60894400	2.81929700	0.01357920
O	−0.01117960	3.78541830	−0.61305380	Zn	−0.04957760	5.65553120	0.00005060
O	1.62013640	6.54748820	−0.57619140	Zn	−0.14887000	3.77059460	2.63982090
O	1.42758450	2.83474970	1.98305970	Zn	1.60141230	6.61468350	2.63036550
O	0.00026380	5.63991090	1.99443280	Zn	1.56964270	2.78301410	5.34953660
O	−0.00096280	3.74736800	4.63754290	O	1.62676680	6.57960240	4.62935030
O	1.59170990	2.79605600	7.35302160	O	1.62813440	8.49231000	1.97916780
Zn	4.86179500	0.90187980	−2.63164130	O	3.23018530	−0.05614430	−3.24518250
O	3.24862560	−1.96544030	−0.66108430	Zn	3.24383000	−0.06340690	−0.01192580
O	4.85157880	0.87703550	−0.65692040	Zn	4.91601620	0.80291550	2.66381680
O	3.24514910	−0.00858790	1.97417050	O	4.89584050	0.94414550	4.66263000
Zn	3.23219410	3.76179570	−2.61764940	O	4.88332760	2.81157940	−3.18780870
Zn	4.87876610	6.58092690	−2.56861090	O	3.24682590	5.65247060	−3.19423580
Zn	4.93429170	2.79442970	−0.22813720	O	3.25530880	3.73613080	−0.60540990
Zn	3.24646200	5.59599590	0.05641870	O	4.87426110	6.54594760	−0.57323790
Zn	2.89750250	3.83006340	2.89686660	O	5.39898890	2.62023600	1.70930680
H	4.52438840	2.78957010	2.19637940	H	3.64145620	2.34700180	3.05193560
Zn	4.86286090	6.57106010	2.64088680	O	3.22339540	5.58400740	2.07222060
Zn	4.82440080	2.82420430	5.26270570	O	3.16429510	3.85349220	4.90889550
Zn	3.24069990	5.73912740	5.37342630	O	4.86216370	6.57103770	4.64189490
O	4.90118760	2.80118800	7.29617400	O	3.25043520	5.67316710	7.37110420
O	4.86959500	8.46751460	1.98732110	O	6.56955900	−0.05389330	1.97522220
Zn	6.52600410	3.78672380	−2.64233680	O	6.53382720	5.68417810	−3.24298280
O	6.55663620	3.81780250	−0.67150570	Zn	6.54980460	5.66421810	−0.00313120
O	8.19676460	6.61298290	−0.65545420	Zn	6.68457200	3.78934370	2.65005200
O	8.23764270	2.76871560	1.96414580	O	6.48997790	5.63554410	1.99416210
O	6.47250130	3.73769490	4.62226250				

calculated wave numbers in cm^{-1} (unscaled):													
82	86	93	95	96	96	100	103	107	110	110	112	112	114
115	115	118	120	121	121	124	126	129	129	131	133	135	136
137	142	142	144	146	146	148	150	154	157	158	159	177	183
184	184	189	192	193	196	198	198	206	209	210	214	215	218
224	225	226	230	233	237	241	245	247	249	251	252	257	268
362	378	414	419	422	427	431	435	436	438	441	441	445	447
448	449	450	451	452	454	454	455	456	458	460	461	463	463
464	466	466	468	469	470	471	473	474	474	475	476	476	478
478	479	480	481	482	483	483	485	486	486	489	490	491	492
494	495	497	498	499	502	503	505	506	506	507	508	510	512
515	516	517	520	521	521	523	524	526	528	529	530	531	532
535	536	537	538	539	540	541	542	544	544	545	546	548	548
550	553	554	557	558	560	563	563	564	565	567	577	580	590
600	649	946	1011	1127	1564	2864							

IR intensities in km/mol:													
0.7	0.6	0.2	0.1	0.2	0.4	0.0	0.3	0.2	0.1	0.1	0.3	0.1	0.3
0.4	0.0	0.1	0.2	0.1	0.2	0.6	0.4	0.2	0.4	0.5	0.2	0.4	0.2
0.2	0.1	0.5	0.3	0.5	0.2	0.6	0.2	0.9	0.3	0.2	0.6	0.3	0.2
1.2	2.7	0.2	0.1	0.5	0.3	0.2	0.2	1.4	1.5	3.6	0.9	0.1	0.4
1.6	0.8	4.5	0.2	0.4	5.7	3.4	2.8	2.4	10.8	4.5	7.5	4.3	10.5
116.0	64.9	9.9	30.9	29.3	44.6	38.9	6.7	19.8	70.9	22.7	2.5	46.9	6.8
127.8	30.2	19.2	34.2	128.9	111.2	108.0	69.8	14.8	2.7	28.4	61.5	22.9	16.2
389.7	120.6	3.9	19.8	14.6	28.3	218.2	25.9	71.4	47.8	63.0	19.0	42.5	20.3
10.6	19.6	83.8	94.8	78.8	97.0	13.1	52.9	75.9	171.6	42.2	23.7	51.4	109.1
188.2	77.2	79.4	61.1	74.1	20.3	38.3	45.6	10.2	18.6	124.3	235.8	171.3	457.5
109.0	41.8	233.4	83.5	237.3	68.4	125.6	29.5	189.3	84.2	275.9	80.2	51.5	22.9
35.8	112.4	84.9	255.7	44.5	215.5	63.8	66.5	50.2	34.2	117.0	72.1	3.4	30.0
50.2	30.4	76.7	119.4	49.6	110.6	48.4	114.2	21.2	46.2	18.0	17.5	7.6	184.8
143.8	1.0	26.2	27.6	219.7	111.9	593.0							

- $2H_{BC_{\parallel}}$

Energy (a.u.)	ZPVE (a.u.)
-154897.8247293	0.1716450

relaxed coordinates in Å:

H	1.39147680	2.67993000	1.62044460	H	0.53518960	2.18401510	0.88998030
O	−1.70900010	6.62357090	−0.65781590	O	−1.67573830	2.79989560	1.99744560
Zn	1.66108030	0.87318030	−2.69508380	O	1.68390760	0.77493290	−0.75081950
Zn	1.59245360	0.82367050	2.72813120	O	−0.03807600	−0.03669680	1.99744950
O	1.62036100	0.93889710	4.70931620	Zn	−0.03814350	3.81625730	−2.69478110
O	1.61654010	2.80959920	−3.18035900	Zn	1.62003250	6.58546700	−2.56999400
O	−0.03170780	5.71350540	−3.26330770	Zn	1.47784700	2.72917220	−0.40879170
O	−0.11122510	3.88499640	−0.75039000	Zn	−0.06243030	5.67581500	0.00165220
O	1.61118910	6.55605350	−0.58220760	Zn	−0.11588410	3.78248650	2.72851380
O	1.72090630	2.87099120	2.59040090	Zn	1.62443060	6.59001810	2.63248400
O	0.01205500	5.61296700	2.00014730	Zn	1.64026370	2.82321770	5.28278830
O	−0.00169370	3.74817880	4.70967300	O	1.64200120	6.56518210	4.63598370
O	1.60500000	2.80297190	7.31315390	O	1.62706040	8.48225130	1.98412790
Zn	4.88846750	0.92453260	−2.56987260	O	3.30749080	−0.06977520	−3.26336520
O	3.25691720	−1.97752120	−0.65801370	Zn	3.25925490	−0.07779990	0.00165670
O	4.85839670	0.93163650	−0.58202170	Zn	4.89434020	0.92593600	2.63223810
O	3.24153090	0.01841720	2.00008260	O	4.88183840	0.95355830	4.63587810
Zn	3.27110880	3.76480040	−2.61852970	O	4.89646670	2.80690420	−3.19294410
Zn	4.89279080	6.57937390	−2.57456080	O	3.25425270	5.65124510	−3.19299700
Zn	4.83575400	2.81414890	0.03094540	O	3.17896870	3.71170880	−0.59905490
Zn	3.23008470	5.59517080	0.03104260	O	4.87432210	6.54142310	−0.58348380
Zn	3.42091050	3.85135820	2.79957020	O	4.90995660	2.81872370	2.03032490
Zn	4.89848330	6.61962380	2.63027010	O	3.27134620	5.65716470	2.03046820
Zn	4.92235820	2.79442770	5.32904970	O	3.30684840	3.78528360	4.79485560
Zn	3.25636560	5.67979970	5.32934750	O	4.86755350	6.57150110	4.63263170
O	4.90625840	2.79828660	7.33463080	O	3.25155020	5.66434210	7.33497230
O	4.87573270	8.49936160	1.97765180	O	6.53468680	−0.01767610	1.98416160
Zn	6.51954960	3.76184460	−2.57460540	O	6.54216260	5.65325690	−3.22980090
O	6.47740800	3.76491080	−0.58347470	Zn	6.53945560	5.65176520	0.00530520
O	8.18740260	6.60313880	−0.65288960	Zn	6.55712520	3.74658430	2.63020570
O	8.17384450	2.78713010	1.97768080	O	6.49531090	5.62620040	1.99909240
O	6.50018290	3.74406480	4.63255730				

calculated wave numbers in cm^{-1} (unscaled):													
68	90	92	93	95	97	98	98	106	107	109	110	112	112
113	114	118	118	120	122	125	129	130	130	133	134	135	136
137	142	143	143	143	146	147	152	153	156	158	158	178	183
185	187	188	192	193	198	199	201	205	209	210	212	215	221
224	224	228	231	233	238	240	242	248	249	252	254	256	275
357	407	417	421	423	423	425	432	434	436	439	443	446	446
447	448	450	450	451	452	453	454	455	457	459	461	462	463
465	465	465	465	465	468	469	470	470	471	473	475	475	477
477	478	479	481	483	483	484	486	486	489	489	490	491	493
494	494	495	496	498	502	503	503	506	508	509	511	513	513
514	515	517	517	518	520	521	522	523	526	529	530	532	533
533	535	537	537	539	541	542	542	545	545	547	549	549	550
551	553	554	555	557	558	560	560	562	566	567	578	581	582
586	724	841	1113	1167	1453	2462							

IR intensities in km/mol:													
0.1	1.4	0.1	0.4	0.8	0.1	0.0	0.0	0.2	0.1	0.0	0.0	0.1	0.0
0.1	0.2	0.1	0.1	0.3	0.3	0.3	0.1	0.1	0.1	0.1	0.2	0.0	0.8
0.2	0.2	0.1	0.1	0.1	0.6	0.6	0.7	1.1	0.6	0.0	0.5	1.3	2.6
0.4	0.4	1.8	0.0	0.1	0.5	0.1	0.0	2.1	1.5	3.3	0.5	0.1	0.1
0.1	0.3	1.8	5.3	0.4	5.6	2.6	0.8	4.1	0.4	5.2	7.4	9.2	28.2
2.9	46.7	86.5	21.0	56.9	49.1	55.2	16.9	0.7	26.7	0.1	2.0	106.5	163.8
31.6	18.4	6.5	16.2	2.7	137.2	187.7	85.3	5.2	71.8	11.0	7.1	4.8	45.3
53.7	190.6	15.1	206.7	17.1	27.6	2.1	84.2	327.2	11.9	48.6	7.2	3.9	23.7
12.8	51.1	7.5	116.3	28.3	41.0	7.7	50.5	174.7	274.2	114.4	74.8	34.0	18.9
186.5	2.9	29.7	152.7	35.1	106.9	89.1	21.9	114.0	1.6	72.2	665.5	36.6	0.4
190.7	9.3	254.1	262.9	160.6	166.8	138.3	28.6	4.9	235.2	48.9	95.9	209.2	55.1
26.3	41.5	313.1	45.4	40.0	80.4	36.5	49.0	16.2	50.7	26.7	80.0	19.6	102.8
40.5	4.8	174.3	162.5	9.3	80.7	32.0	0.7	29.9	20.5	51.1	80.0	231.4	72.7
149.4	22.9	95.4	23.4	305.5	102.2	728.8							

- $H_{BC_{\parallel}}$-$H_{AB_{\parallel}}$

Energy (a.u.)	ZPVE (a.u.)
-154897.8058387	0.1732290

relaxed coordinates in Å:

H	1.39778990	2.69882610	1.20157090	H	2.99029870	3.59322050	0.66546140
O	−1.69283950	6.60493180	−0.65750480	O	−1.65793440	2.79141730	1.97986360
Zn	1.66195260	0.77943940	−2.63567330	O	1.66120750	0.89710130	−0.61256590
Zn	1.60564500	0.81540020	2.70396870	O	−0.03658070	−0.01696080	1.97978440
O	1.61802600	0.95921960	4.67022180	Zn	−0.11824890	3.86341810	−2.63584460
O	1.59846950	2.79853210	−3.10166920	Zn	1.61092740	6.59953920	−2.57067770
O	−0.03518600	5.70754650	−3.25830290	Zn	1.60579410	2.80225240	−0.95702670
O	−0.01635430	3.80346490	−0.61235750	Zn	−0.05305180	5.67629820	0.03616930
O	1.60099560	6.55194030	−0.59431360	Zn	−0.11922850	3.79898820	2.70829630
O	1.60438400	2.80512290	2.16076320	Zn	1.62221670	6.61166880	2.66297570
O	0.01919540	5.62858040	2.01645010	Zn	1.61031780	2.80511220	5.34120650
O	0.01496100	3.73572000	4.67293870	O	1.64087670	6.56275860	4.65555570
O	1.60009410	2.80003170	7.33905880	O	1.62732420	8.48519870	1.97972470
Zn	4.89611160	0.90902550	−2.57068900	O	3.30067170	−0.07005460	−3.25847940
O	3.24886570	−1.95460020	−0.65782350	Zn	3.26479590	−0.07038140	0.03597040
O	4.85002260	0.92432580	−0.59433210	Zn	4.91177410	0.91337450	2.66265510
O	3.25916740	0.01654290	2.01588380	O	4.87933480	0.95359190	4.65532560
Zn	3.31236610	3.78780970	−2.90752510	O	4.92879560	2.79731090	−3.18637830
Zn	4.92850390	6.59493990	−2.58137310	O	3.26236260	5.68283590	−3.18622650
Zn	5.03910080	2.74651910	0.07099110	O	3.25599570	3.75383630	−0.27949250
Zn	3.27241860	5.80080410	0.07137550	O	4.92716590	6.55927090	−0.60281450
Zn	3.35720030	3.81525080	2.81814050	O	4.87887950	2.81155970	2.05302220
Zn	4.89207460	6.61143800	2.65771820	O	3.24956430	5.63442050	2.05354210
Zn	4.90521470	2.79738170	5.33066500	O	3.25056420	3.75255430	4.76675060
Zn	3.25052170	5.66314910	5.33106830	O	4.85763930	6.56342050	4.65179160
O	4.89985980	2.79994650	7.33359990	O	3.24978660	5.65788450	7.33410580
O	4.87229380	8.48578840	1.97925070	O	6.53730620	−0.01881590	1.97985990
Zn	6.55093600	3.78515100	−2.58179280	O	6.55012700	5.65797550	−3.24520030
O	6.52051740	3.80295670	−0.60315580	Zn	6.57556270	5.67323280	0.03588740
O	8.20185680	6.61157840	−0.65921930	Zn	6.54651450	3.74527990	2.65773720
O	8.16000180	2.79119040	1.97932830	O	6.48709360	5.62153010	2.01626780
O	6.48815310	3.73946530	4.65164750				

calculated wave numbers in cm^{-1} (unscaled):													
52	78	85	87	90	93	93	95	97	100	103	104	106	107
109	110	111	112	116	117	119	121	122	128	129	131	132	133
135	137	139	139	140	142	143	149	151	152	156	157	158	173
183	185	186	188	192	193	194	196	198	202	204	210	212	219
221	223	224	225	230	238	241	242	245	247	248	255	258	261
282	356	359	379	382	393	394	407	415	417	421	430	439	440
441	442	443	447	450	451	453	455	455	457	458	458	459	460
461	464	464	465	466	466	467	468	468	470	471	471	472	475
475	477	478	479	480	480	481	483	484	484	485	487	487	488
490	490	493	494	494	495	498	499	500	502	503	503	505	506
507	508	509	510	511	514	516	517	518	518	520	522	523	524
525	528	528	529	531	532	534	535	537	537	540	542	543	544
546	548	549	551	552	554	556	557	560	561	564	564	572	578
579	581	667	697	903	3338	3466							

IR intensities in km/mol:													
0.4	0.7	0.1	0.1	0.0	0.0	0.1	1.0	0.3	0.1	0.1	0.1	2.2	0.0
0.2	0.5	0.2	0.0	0.0	0.0	0.4	0.1	0.8	0.2	0.1	0.5	0.2	0.0
0.1	1.4	0.1	0.3	0.1	0.1	0.0	1.4	0.3	0.8	0.3	0.1	0.1	1.5
2.5	1.0	0.1	0.7	0.1	0.1	0.4	0.0	0.2	0.0	0.8	0.1	0.1	0.0
0.3	0.2	0.2	0.7	0.7	3.0	0.1	1.2	5.2	6.5	5.5	19.5	14.5	8.8
0.1	5.6	9.6	17.9	16.6	32.5	14.2	9.9	0.5	112.5	36.9	0.8	11.6	16.7
13.7	2.6	25.7	1.2	1.5	3.3	24.1	83.1	57.0	36.5	31.8	7.5	111.3	2.0
36.5	4.8	40.5	137.1	20.2	27.0	126.0	157.5	5.7	6.3	5.5	22.9	0.6	67.5
54.3	65.4	7.9	74.6	76.3	35.9	14.4	1.6	21.7	4.5	81.6	26.5	11.4	2.4
21.1	11.6	1.1	24.5	5.0	4.6	3.0	0.3	34.7	29.8	1.5	20.9	64.3	107.8
136.5	44.2	45.6	1.3	71.2	8.0	18.8	1.7	21.9	19.8	175.3	55.8	18.3	55.2
41.7	10.5	14.6	9.2	6.2	0.0	9.9	6.3	6.6	16.3	0.0	0.2	2.3	0.3
18.7	12.2	22.7	32.8	6.5	0.8	2.5	6.5	46.4	13.4	48.6	17.8	17.4	34.1
32.1	1.6	2.2	1.0	2.3	15.8	156.9							

2.2 Hydrogen Complexes at Zinc or Oxygen Vacancies

- H_2-V_O^{2+}

Energy (a.u.)	ZPVE (a.u.)
-154822.7928510	0.1650745

relaxed coordinates in Å:

H	3.00000000	3.00000000	−0.00000000	H	3.00000000	3.00000000	−0.00000000
O	−1.00000000	6.00000000	−0.00000000	O	−1.00000000	2.00000000	1.00000000
Zn	1.00000000	0.00000000	−2.00000000	O	1.00000000	0.00000000	−0.00000000
Zn	1.00000000	0.00000000	2.00000000	O	−0.00000000	0.00000000	1.00000000
O	1.00000000	0.00000000	4.00000000	Zn	−0.00000000	3.00000000	−2.00000000
O	1.00000000	2.00000000	−3.00000000	Zn	1.00000000	6.00000000	−2.00000000
O	−0.00000000	5.00000000	−3.00000000	Zn	1.00000000	2.00000000	0.00000000
O	0.00000000	3.00000000	−0.00000000	Zn	−0.00000000	5.00000000	0.00000000
O	1.00000000	6.00000000	−0.00000000	Zn	−0.00000000	3.00000000	2.00000000
O	1.00000000	2.00000000	2.00000000	Zn	1.00000000	6.00000000	2.00000000
O	0.00000000	5.00000000	2.00000000	Zn	1.00000000	2.00000000	5.00000000
O	0.00000000	3.00000000	4.00000000	O	1.00000000	6.00000000	4.00000000
O	1.00000000	2.00000000	7.00000000	O	1.00000000	8.00000000	1.00000000
Zn	4.00000000	0.00000000	−2.00000000	O	3.00000000	−0.00000000	−3.00000000
O	3.00000000	−1.00000000	−0.00000000	Zn	3.00000000	−0.00000000	0.00000000
O	4.00000000	0.00000000	−0.00000000	Zn	4.00000000	0.00000000	2.00000000
O	3.00000000	0.00000000	2.00000000	O	4.00000000	0.00000000	4.00000000
Zn	3.00000000	3.00000000	−3.00000000	O	4.00000000	2.00000000	−3.00000000
Zn	4.00000000	6.00000000	−2.00000000	O	3.00000000	5.00000000	−3.00000000
Zn	5.00000000	2.00000000	0.00000000	Zn	3.00000000	6.00000000	0.00000000
O	4.00000000	6.00000000	−0.00000000	Zn	3.00000000	3.00000000	2.00000000
O	4.00000000	2.00000000	2.00000000	Zn	4.00000000	6.00000000	2.00000000
O	3.00000000	5.00000000	2.00000000	Zn	4.00000000	2.00000000	5.00000000
O	3.00000000	3.00000000	4.00000000	Zn	3.00000000	5.00000000	5.00000000
O	4.00000000	6.00000000	4.00000000	O	4.00000000	2.00000000	7.00000000
O	3.00000000	5.00000000	7.00000000	O	4.00000000	8.00000000	1.00000000
O	6.00000000	0.00000000	1.00000000	Zn	6.00000000	3.00000000	−2.00000000
O	6.00000000	5.00000000	−3.00000000	O	6.00000000	3.00000000	−0.00000000
Zn	6.00000000	5.00000000	0.00000000	O	8.00000000	6.00000000	−0.00000000
Zn	6.00000000	3.00000000	2.00000000	O	8.00000000	2.00000000	1.00000000
O	6.00000000	5.00000000	2.00000000	O	6.00000000	3.00000000	4.00000000

calculated wave numbers in cm^{-1} (unscaled):													
80	84	89	93	93	93	97	100	102	104	104	108	111	111
113	114	114	115	116	121	122	124	124	127	131	134	134	136
136	139	139	141	142	143	144	146	151	151	160	160	162	185
186	187	189	197	199	199	201	201	206	207	212	214	221	222
227	229	229	230	235	238	241	241	246	249	254	258	261	262
272	351	378	380	387	395	396	400	406	415	416	418	420	422
426	430	432	438	449	450	451	452	455	457	457	460	461	461
464	465	465	465	471	471	473	473	474	475	475	476	478	479
480	481	481	482	483	484	484	487	487	490	492	493	493	494
495	498	498	499	501	501	502	502	503	505	507	507	507	511
511	514	515	515	516	519	523	523	524	525	525	530	530	530
535	535	538	539	539	539	544	544	545	545	547	549	549	553
554	554	569	569	569	575	577	580	589	590	600	600	602	604
608	610	615	3975										

IR intensities in km/mol:													
2.1	1.6	0.9	0.0	0.1	0.0	3.2	0.1	0.0	0.1	0.1	0.0	0.1	0.1
0.4	0.0	0.1	0.0	0.2	0.4	0.3	0.0	0.1	0.0	0.0	0.1	0.1	0.1
0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.0	1.2	1.4	0.4	0.3	0.0	0.6
2.0	3.3	0.1	0.7	0.2	0.0	0.0	0.0	0.1	1.6	0.3	0.3	0.6	0.1
3.5	0.1	0.2	1.6	0.5	0.7	1.4	0.4	1.7	0.5	0.1	11.4	16.6	12.9
14.7	31.0	2.1	7.0	0.0	1.0	1.4	243.2	1.1	21.5	18.6	3.4	5.9	199.3
167.8	13.6	9.2	1.3	0.2	11.5	9.0	1.2	0.2	11.4	12.9	0.2	0.5	0.6
0.0	0.2	21.6	60.9	0.9	0.7	1.1	11.3	110.6	96.3	79.7	53.2	0.1	150.9
77.1	64.2	8.1	7.6	0.0	268.9	289.9	367.5	336.3	264.9	0.5	76.8	59.6	37.3
64.9	44.5	67.2	150.7	100.2	139.0	111.7	107.4	191.6	16.0	160.7	298.9	251.6	19.8
48.8	211.0	5.5	54.8	39.7	0.0	4.7	0.1	559.0	296.3	294.0	245.1	17.3	13.6
0.0	15.2	1.4	19.4	38.6	62.6	20.9	26.4	28.5	1.9	17.4	0.4	0.1	0.2
83.7	89.9	67.8	79.8	76.0	9.7	3.4	0.3	100.4	81.0	268.1	265.2	30.9	93.7
117.7	30.6	206.8	5.0										

- $H_{BC_\perp}$-V_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153118.0280089	0.1624386

relaxed coordinates in Å:

H	4.04616950	3.29216090	2.40182550	O	−1.69296830	6.60633500	−0.65628890
O	−1.65868650	2.79552520	1.98202310	Zn	1.62296400	0.92457330	−2.58842720
O	1.64574040	0.93506230	−0.60469060	Zn	1.60264940	0.93916600	2.64932760
O	−0.03468430	−0.02501190	1.98029790	O	1.61987850	0.94566030	4.64058200
Zn	−0.01768880	3.76519350	−2.58488380	O	1.60325280	2.80378540	−3.20416870
Zn	1.60518120	6.57606040	−2.58513320	O	−0.04462960	5.65456360	−3.23813800
Zn	1.62906430	2.82856700	0.03635500	O	−0.00124470	3.77799260	−0.60504060
Zn	−0.04709790	5.65618920	0.01464250	O	1.60211540	6.55564870	−0.60548300
Zn	0.00660740	3.74489260	2.63709410	O	1.53074270	2.74585420	1.96634390
Zn	1.63536970	6.56488280	2.63670570	O	0.00351820	5.62689070	2.00191330
Zn	1.65005690	2.83601640	5.25889470	O	0.00463050	3.73922570	4.63751570
O	1.63899580	6.56986150	4.63733980	O	1.59492330	2.79569740	7.30755170
O	1.62456830	8.48201270	1.98200320	Zn	4.87434100	0.91947220	−2.57926530
O	3.25259810	−0.04878830	−3.23109480	O	3.25136540	−1.95157070	−0.65447920
Zn	3.23953730	−0.05214110	0.00743640	O	4.85381740	0.94012730	−0.57971780
Zn	4.86845310	0.88553790	2.66475150	O	3.24255790	0.00588890	1.99637380
O	4.88839120	0.95243270	4.64058550	Zn	3.24064610	3.75790850	−2.64261530
O	4.89339350	2.80383070	−3.19115280	Zn	4.88574990	6.57556230	−2.58869960
O	3.24833860	5.65291780	−3.20421390	Zn	4.83479550	2.83768570	−0.03487750
O	3.22660050	3.76599470	−0.64726310	Zn	3.23977450	5.61867050	0.03535040
O	4.88818500	6.55085950	−0.60515480	O	4.84446970	2.83174610	2.02796050
Zn	4.86244100	6.58557500	2.64910510	O	3.26226030	5.74486150	1.96498310
Zn	4.86221910	2.82173970	5.30911310	O	3.27497320	3.73814050	4.76009070
Zn	3.24375150	5.59648970	5.25849230	O	4.86585900	6.56773740	4.64044210
O	4.91069340	2.79390350	7.33345120	O	3.25124020	5.66446800	7.30750600
O	4.87934980	8.48580700	1.98027480	O	6.52160340	−0.00408050	1.98429290
Zn	6.51580760	3.76246680	−2.57925190	O	6.54369610	5.65101280	−3.23114960
O	6.48768000	3.76992620	−0.57970990	Zn	6.53973950	5.66409240	0.00748400
O	8.19075860	6.60348940	−0.65434860	Zn	6.54206730	3.78466020	2.66481490
O	8.13922640	2.79782980	1.98436860	O	6.49104660	5.63250020	1.99643570
O	6.49416330	3.73388510	4.64063470				

calculated wave numbers in cm^{-1} (unscaled):													
89	91	94	96	98	99	103	104	105	109	111	112	113	116
116	117	118	121	122	125	126	127	127	128	128	130	130	135
138	138	140	144	144	147	147	149	150	158	158	159	163	182
183	183	190	192	196	197	198	198	203	210	210	213	215	216
225	226	230	231	238	238	243	248	249	250	302	303	323	345
385	398	400	409	429	432	434	435	437	442	442	443	445	446
448	449	451	452	453	453	454	457	457	458	460	461	461	464
465	465	466	468	469	470	471	472	473	474	474	475	476	478
479	480	480	481	483	483	484	485	485	488	489	490	491	491
493	494	495	497	498	499	502	504	505	507	509	510	510	511
514	515	516	518	518	520	521	522	522	525	525	527	529	532
532	533	534	535	536	537	538	539	541	542	542	545	546	547
549	552	553	553	556	557	560	563	570	572	588	598	835	869
3435													

IR intensities in km/mol:													
3.1	0.7	0.0	0.0	1.2	0.3	1.2	0.1	0.1	0.2	0.0	0.4	0.1	0.0
1.0	0.1	0.1	1.8	0.1	0.7	0.1	0.5	0.4	0.2	0.0	0.1	0.1	0.0
0.8	1.8	0.2	0.2	1.0	0.4	1.1	1.3	2.3	0.1	0.1	0.2	0.9	0.4
1.9	0.1	0.0	0.1	0.0	0.6	0.5	0.5	5.2	2.9	3.3	1.6	0.5	0.4
1.4	1.5	4.5	0.1	3.2	3.5	3.2	11.6	12.7	2.9	27.7	18.6	15.2	4.0
46.2	23.1	25.9	54.4	5.1	15.8	12.2	0.6	4.0	20.1	3.9	427.2	1.6	9.9
117.6	0.1	81.8	6.1	169.1	14.6	104.8	52.7	94.4	27.6	236.1	37.4	35.2	32.0
9.7	98.4	13.9	2.2	28.1	184.5	60.0	9.4	35.7	76.7	0.9	28.8	57.8	14.6
3.5	60.7	28.7	1.5	39.1	33.5	69.4	81.2	58.5	12.6	8.3	57.5	3.8	38.7
80.2	69.9	9.9	22.8	54.1	24.1	23.9	52.3	102.5	388.3	9.5	167.3	58.1	26.4
126.9	204.6	152.8	3.9	101.4	199.9	122.1	120.0	167.4	36.3	105.9	64.0	46.1	21.8
1.6	71.7	47.7	264.6	24.3	6.8	55.7	31.3	41.9	5.1	74.7	14.7	4.3	60.6
42.6	6.4	19.3	9.7	18.5	13.3	0.1	16.6	29.7	69.7	54.8	43.9	3.6	3.9
120.8													

- $H_{BC_{\parallel}}$-V_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153118.0259613	0.1628504

relaxed coordinates in Å:

H	4.87663350	2.84789890	0.94775480	O	−1.68739680	6.60455190	−0.65138970
O	−1.66576080	2.79003000	1.98376190	Zn	1.63438880	0.92638960	−2.59381620
O	1.62670400	0.92338380	−0.59718340	Zn	1.59003940	0.91647590	2.63651770
O	−0.04341280	−0.02392210	1.98383040	O	1.62102220	0.95044710	4.64279720
Zn	0.00201860	3.75350340	−2.58607270	O	1.63223560	2.81170580	−3.19289810
Zn	1.62575940	6.56576210	−2.58150470	O	−0.03867080	5.65479450	−3.22825360
Zn	1.64208720	2.80901070	0.01236110	O	−0.00359330	3.76751090	−0.59082530
Zn	−0.03451600	5.64960490	−0.00212880	O	1.62394720	6.55321020	−0.58585370
Zn	−0.03660050	3.74546750	2.62825450	O	1.60091110	2.79947810	2.02959150
Zn	1.61444700	6.60146290	2.62778100	O	0.00759680	5.62546350	1.99742850
Zn	1.62078750	2.81249310	5.27646150	O	0.01003910	3.74193940	4.63706050
O	1.63932330	6.56376230	4.63635710	O	1.60441860	2.80162190	7.30027020
O	1.62544990	8.49077560	1.98201380	Zn	4.88925600	0.94755870	−2.52466200
O	3.26492110	−0.04482620	−3.22705560	O	3.24750170	−1.95569410	−0.65033910
Zn	3.23646430	−0.03645580	−0.00656510	O	4.85360290	0.84387590	−0.58064890
Zn	4.88858930	0.87881880	2.59175590	O	3.23059860	0.00607550	1.99807400
O	4.88021990	0.95721220	4.59667600	Zn	3.29655510	3.72958290	−2.53078370
O	4.90244700	2.79542640	−3.20935390	Zn	4.89973130	6.56712780	−2.58826790
O	3.25993920	5.62533910	−3.18850340	O	3.19806040	3.77090420	−0.58012390
Zn	3.28243150	5.60194680	0.01706540	O	4.89580590	6.56743200	−0.59428160
Zn	3.19726740	3.78229670	2.63214240	O	4.87749850	2.81922740	1.94520570
Zn	4.87898420	6.60850620	2.63713800	O	3.25226840	5.65623130	2.02989400
Zn	4.89043250	2.80707970	5.27865120	O	3.26190910	3.74482820	4.64444680
Zn	3.24958400	5.63304390	5.27653890	O	4.86100210	6.56455730	4.64384890
O	4.90029240	2.79952900	7.29603230	O	3.25055810	5.65300850	7.30057560
O	4.87238620	8.49365260	1.98305680	O	6.54390680	−0.02374330	1.98576420
Zn	6.50469460	3.73719220	−2.49728420	O	6.54511230	5.63551220	−3.22694250
O	6.55237770	3.79045650	−0.55359860	Zn	6.53689170	5.63217920	−0.00719610
O	8.19370480	6.61255520	−0.65086840	Zn	6.56896460	3.77488290	2.59073150
O	8.17108210	2.78296180	1.99240430	O	6.48454230	5.64594370	2.00247450
O	6.48652170	3.73839000	4.59861400				

calculated wave numbers in cm^{-1} (unscaled):													
86	95	96	97	98	100	104	106	107	110	111	112	113	114
116	119	121	121	124	126	127	133	134	135	135	137	138	140
140	143	145	145	145	146	151	151	152	158	159	160	163	181
185	187	191	193	194	195	198	199	201	208	210	214	215	223
224	226	229	231	233	240	241	243	248	254	301	311	333	356
397	404	417	423	430	433	433	436	437	439	440	441	443	445
447	449	450	451	452	453	453	457	457	458	459	461	462	463
465	465	466	468	468	469	470	471	472	473	473	475	476	477
477	478	479	481	482	483	485	486	488	490	491	491	492	494
495	497	499	499	500	501	502	503	503	505	510	512	513	515
515	516	518	519	519	521	524	525	527	527	529	530	531	531
534	534	537	538	539	540	542	544	544	545	546	547	548	549
551	552	554	555	556	558	559	563	568	570	570	581	862	884
3379													

IR intensities in km/mol:													
0.3	0.7	0.2	0.1	0.0	0.1	0.3	0.8	0.0	0.8	0.7	0.4	0.2	0.1
0.2	1.7	0.2	0.3	0.0	0.4	0.3	0.1	0.8	0.4	0.2	0.3	0.6	0.1
0.1	0.2	0.2	0.6	0.4	0.7	1.2	0.7	0.9	0.7	0.1	0.1	1.8	3.7
0.1	1.7	0.1	0.4	1.1	2.3	0.1	0.5	2.4	2.2	2.3	0.9	1.0	2.0
1.0	4.6	0.9	2.2	1.9	5.0	3.9	4.0	5.5	3.4	11.2	15.7	14.9	3.4
54.6	43.1	1.2	74.5	0.3	91.4	22.2	10.4	17.8	63.1	37.4	22.9	38.6	25.2
49.0	85.3	25.5	4.3	15.0	82.5	221.2	48.8	238.4	130.9	40.0	44.2	9.7	249.8
93.3	3.0	38.5	78.8	22.1	22.8	93.8	5.9	128.8	61.3	14.8	32.7	55.3	28.4
9.5	9.6	63.3	4.8	41.8	30.2	232.9	97.4	17.6	84.1	19.5	21.6	71.3	48.5
45.1	55.3	18.3	43.9	0.7	127.0	146.4	60.7	99.6	242.2	139.7	208.6	176.8	55.6
54.9	61.3	99.5	33.3	85.5	22.0	191.0	67.2	195.3	103.3	20.6	20.8	15.8	28.0
10.7	275.9	62.1	66.1	16.5	1.4	59.5	57.4	26.0	7.5	59.6	49.5	13.7	41.0
64.2	13.3	5.9	9.2	16.7	2.1	13.4	29.9	3.3	112.7	116.3	5.5	14.9	10.0
212.4													

- $H_{AB_{\perp}}$-V_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153117.9901426	0.1637049

relaxed coordinates in Å:

H	1.96443290	4.49438450	−1.04092360	O	−1.68980720	6.60454280	−0.65330050
O	−1.65967820	2.79422450	1.98039610	Zn	1.64046100	0.90653740	−2.59553990
O	1.64848320	0.89143040	−0.60351950	Zn	1.60735340	0.90036130	2.66784590
O	−0.03719930	−0.01441720	1.98275020	O	1.61484390	0.95458480	4.65995230
Zn	−0.01681560	3.74884340	−2.58813470	O	1.60723290	2.79718260	−3.20187520
Zn	1.61976720	6.58344310	−2.58814320	O	−0.03704510	5.65022870	−3.22372190
Zn	1.57075250	2.68239370	0.12566000	O	0.01318080	3.76957850	−0.58584520
Zn	−0.05438110	5.66058920	0.02524940	O	1.61717660	6.54723140	−0.58612520
Zn	−0.03663910	3.74681830	2.65486510	O	1.61034210	2.80506770	2.07635160
Zn	1.61172310	6.60169120	2.65495160	O	0.00911620	5.62372680	2.00961360
Zn	1.61568640	2.81043340	5.30400100	O	0.00676930	3.74203270	4.64921400
O	1.63766980	6.56652060	4.64928750	O	1.59926390	2.80151800	7.31833470
O	1.62522390	8.48352570	1.98038420	Zn	4.89056540	0.92607590	−2.53548070
O	3.25882710	−0.04871810	−3.23949620	O	3.24140330	−1.98088950	−0.65872340
Zn	3.26235500	−0.08228390	0.02306490	O	4.84283710	0.77924960	−0.61356850
Zn	4.90257030	0.92494250	2.58523830	O	3.23317710	0.00271180	2.01166110
O	4.87697740	0.93682670	4.62269840	Zn	3.29856800	3.72450780	−2.74043390
O	4.91795720	2.78985320	−3.20929940	Zn	4.91008730	6.56942270	−2.59551620
O	3.25605540	5.65295940	−3.20180030	O	2.78942000	4.01800920	−0.77745970
Zn	3.33700060	5.74149940	0.12542540	O	4.92665210	6.57013490	−0.60362090
Zn	3.25985870	3.74699410	2.68789950	O	4.87191270	2.81665430	2.17534530
Zn	4.89861830	6.60114140	2.66781670	O	3.25057000	5.64630760	2.07605320
Zn	4.89934020	2.80043350	5.25507730	O	3.24052900	3.75810250	4.70684740
Zn	3.24887740	5.63904190	5.30428890	O	4.85557710	6.56763620	4.65991980
O	4.89849130	2.80096960	7.29169800	O	3.24841330	5.65790520	7.31866570
O	4.86885050	8.48272760	1.98272450	O	6.54686430	−0.02985080	1.98394360
Zn	6.51835590	3.74531710	−2.53523370	O	6.54671390	5.64576770	−3.23953670
O	6.62233110	3.86054430	−0.61337170	Zn	6.57716200	5.65991450	0.02314190
O	8.21125800	6.62690500	−0.65855520	Zn	6.52560660	3.73566930	2.58539680
O	8.17429570	2.78884340	1.98392610	O	6.48908500	5.64230900	2.01169460
O	6.50213900	3.75162300	4.62276830				

calculated wave numbers in cm^{-1} (unscaled):													
88	93	94	95	96	97	103	103	104	106	108	109	112	112
113	117	119	120	121	127	127	129	131	131	134	134	135	137
138	139	142	143	143	146	148	149	152	157	158	160	179	184
186	187	192	193	195	196	199	200	203	210	212	216	218	221
224	227	231	233	236	239	243	247	250	254	280	297	299	315
410	415	415	421	424	425	432	439	439	442	444	445	446	447
449	449	451	453	454	454	457	459	460	460	461	462	464	465
465	468	468	469	469	471	471	473	473	476	476	477	479	480
480	480	482	482	485	486	488	489	489	490	492	492	494	496
496	498	500	503	504	505	508	508	511	512	513	513	518	519
520	520	522	525	526	526	529	530	531	531	533	533	534	536
537	540	541	541	542	543	544	545	546	548	548	551	552	552
553	555	557	560	560	563	567	572	573	577	580	589	894	930
3476													

IR intensities in km/mol:													
0.2	0.0	0.5	0.2	0.0	0.3	0.3	0.1	0.4	0.0	0.1	0.6	0.1	0.3
0.0	0.7	0.1	0.3	0.1	0.2	0.3	0.3	1.2	1.2	1.2	0.2	0.4	0.0
0.0	0.1	0.2	0.1	0.1	0.7	1.7	1.9	0.8	1.1	1.3	1.1	1.0	0.5
0.1	5.5	0.7	0.2	1.6	0.2	0.9	0.1	0.4	0.5	2.4	1.7	0.0	3.6
2.2	1.2	0.0	0.1	4.7	3.8	5.8	2.1	16.3	9.1	4.1	22.3	43.7	7.4
13.6	70.4	1.4	9.0	52.1	13.9	0.1	20.4	2.1	6.4	68.2	5.5	90.2	146.8
74.0	254.3	79.0	23.2	20.5	24.5	29.3	11.8	410.0	258.2	0.8	63.8	35.9	143.7
90.3	0.2	104.2	19.0	67.9	1.9	0.9	10.9	40.6	24.8	28.0	56.4	140.2	26.7
16.9	9.4	34.0	0.9	59.0	33.6	120.5	7.2	0.3	22.3	26.2	10.4	165.3	42.5
32.8	0.1	97.0	4.6	132.9	265.6	150.5	241.7	373.5	13.5	203.4	130.5	1.4	58.4
198.2	69.8	2.1	49.4	209.3	86.6	0.0	252.7	38.3	27.6	8.5	92.2	66.9	37.3
13.2	23.9	10.4	26.6	167.0	96.0	31.1	36.0	72.1	221.4	85.1	14.6	27.5	27.1
88.0	20.3	18.9	41.0	5.9	15.9	65.1	81.5	70.5	148.1	13.3	29.7	91.5	50.9
67.0													

- $H_{AB_{\parallel}}$-V_{Zn}, transition state

Energy (a.u.)	ZPVE (a.u.)
-153117.9835972	0.1629859

relaxed coordinates in Å:

H	4.89273760	2.80190130	3.37862710	O	−1.68835890	6.60367540	−0.65077130
O	−1.67370590	2.78776520	1.98150500	Zn	1.63902260	0.91572040	−2.59843850
O	1.62371520	0.91748730	−0.60191240	Zn	1.58043630	0.91717470	2.63820020
O	−0.04814450	−0.02355950	1.98457890	O	1.62089240	0.95292600	4.64378160
Zn	−0.00042190	3.75251340	−2.58709300	O	1.62628200	2.80700250	−3.19402660
Zn	1.62463440	6.56742940	−2.58712240	O	−0.04061080	5.65221150	−3.22761600
Zn	1.64322410	2.79049110	0.00232790	O	0.00077900	3.76540070	−0.59070650
Zn	−0.03497340	5.64906420	−0.00688830	O	1.61404820	6.56013390	−0.59084500
Zn	−0.05888020	3.74951860	2.62846780	O	1.57105380	2.79788390	2.01775360
Zn	1.59808750	6.61965180	2.62854290	O	0.00574200	5.62557380	1.99569290
Zn	1.62057250	2.81268170	5.28028430	O	0.01166690	3.74212550	4.63582910
O	1.64005900	6.56222610	4.63587960	O	1.60586860	2.80174310	7.30310300
O	1.62379350	8.49889770	1.98146120	Zn	4.89076990	0.94178180	−2.52227230
O	3.26038320	−0.04822770	−3.23410700	O	3.24169250	−1.98265430	−0.65587240
Zn	3.23338730	−0.06185310	−0.02885840	O	4.84620870	0.78252900	−0.59356750
Zn	4.87770930	0.78547810	2.55269770	O	3.20107930	−0.00633440	1.98697050
O	4.88080170	0.96897930	4.61459100	Zn	3.29065060	3.72903300	−2.56198780
O	4.89742580	2.80162710	−3.21071360	Zn	4.90114480	6.56606660	−2.59854290
O	3.25685910	5.63141180	−3.19401600	O	3.15225930	3.80917450	−0.62104480
Zn	3.27955530	5.62540130	0.00214680	O	4.89197210	6.57877880	−0.60208810
Zn	3.10442530	3.83687480	2.61627280	O	4.86639350	2.81913060	2.39413230
Zn	4.87075520	6.61599950	2.63813830	O	3.23714380	5.68421410	2.01750050
Zn	4.89379240	2.80352150	5.38611440	O	3.27228020	3.73963090	4.66878490
Zn	3.24942320	5.63356850	5.28042370	O	4.86009600	6.56324020	4.64369370
O	4.90020960	2.79996680	7.35537450	O	3.25150080	5.65203980	7.30332560
O	4.87134380	8.49670860	1.98451370	O	6.55963350	−0.03289330	1.98660970
Zn	6.50476230	3.73754310	−2.52338910	O	6.54693500	5.64457750	−3.23439460
O	6.62371630	3.85783090	−0.59534770	Zn	6.54524410	5.67564930	−0.02849080
O	8.21326450	6.62783030	−0.65578840	Zn	6.63297870	3.82647660	2.55390720
O	8.18267520	2.77946140	1.98665240	O	6.48086000	5.67416240	1.98702050
O	6.47597300	3.73199310	4.61496790				

calculated wave numbers in cm^{-1} (unscaled):													
58	84	89	94	97	98	100	105	107	108	109	111	112	113
114	117	118	121	123	125	125	129	132	133	134	136	137	138
141	142	143	146	148	151	152	154	156	158	163	163	176	178
180	190	191	194	195	197	199	207	208	211	215	215	222	223
225	226	230	235	237	240	241	249	250	258	266	305	320	360
376	385	388	416	428	429	433	434	436	441	443	443	444	446
447	448	451	452	453	454	456	458	459	460	461	463	463	466
467	468	469	470	472	473	474	475	476	478	478	478	479	480
481	482	485	485	488	489	490	491	494	494	495	497	500	500
501	503	504	506	508	509	510	511	513	514	515	516	518	519
520	521	522	524	526	527	528	530	530	532	534	538	539	541
542	543	544	545	546	547	548	548	551	552	554	556	557	558
561	563	564	569	571	572	582	583	586	633	704	794	817	3528

IR intensities in km/mol:													
203.9	14.4	4.0	3.4	1.3	6.1	3.0	18.1	3.8	2.9	5.0	6.4	3.5	3.2
8.9	6.6	0.6	3.5	2.1	0.6	1.2	6.2	7.3	5.5	3.0	1.1	2.1	0.7
3.9	2.9	5.7	0.3	0.9	0.8	17.8	3.0	11.0	1.8	1.8	1.8	1.8	14.8
24.8	8.3	7.8	10.3	11.0	5.5	5.2	8.6	2.0	2.7	8.7	3.1	36.9	22.9
17.7	2.4	7.4	12.7	35.7	5.2	30.4	80.5	45.4	23.2	238.6	24.8	0.6	328.8
293.2	4.7	4.8	4.6	10.0	0.8	137.3	23.2	254.7	85.4	125.3	22.2	61.4	87.1
26.0	53.2	62.0	165.3	72.1	22.9	12.9	75.1	44.1	24.9	68.2	96.1	16.9	19.3
9.6	21.9	8.9	0.8	10.1	29.6	31.2	49.4	37.4	46.7	17.4	48.1	1.2	84.2
137.6	148.2	31.5	19.4	41.6	55.6	136.2	73.4	61.9	16.5	100.7	36.9	16.7	58.8
110.4	214.9	58.8	150.1	29.1	141.7	85.2	71.1	138.7	196.8	182.6	253.6	71.1	21.4
100.3	63.7	56.3	11.9	128.2	231.0	120.8	6.1	33.2	95.1	118.7	35.5	31.9	3.5
7.7	67.5	59.5	98.9	41.0	22.9	43.3	153.4	12.9	105.5	78.8	32.8	3.7	7.9
15.8	192.9	26.8	113.5	25.9	2.2	129.7	51.5	25.8	1307.5	2113.8	61.7	35.1	87.1

- $H_{BC_\perp}$-$H_{BC_\parallel}$-V_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153118.6990159	0.1736753

relaxed coordinates in Å:

H	3.24976970	4.63390740	2.09560330	H	3.25022180	3.50937590	3.68884560
O	−1.69323560	6.60866790	−0.65416160	O	−1.66470920	2.79579920	1.98591490
Zn	1.62445940	0.92244680	−2.55975030	O	1.64456770	0.94847720	−0.57235330
Zn	1.62937880	0.99056900	2.60251130	O	−0.02613970	−0.01083610	1.98990680
O	1.62066270	0.93634800	4.63783480	Zn	−0.00715150	3.74366690	−2.56494800
O	1.60561000	2.79842990	−3.20498990	Zn	1.59996470	6.56891210	−2.59881260
O	−0.04820790	5.64379510	−3.23005950	Zn	1.66007270	2.82306860	0.14421350
O	0.02238380	3.75753540	−0.57781000	Zn	−0.05722190	5.63473460	−0.00282800
O	1.59251850	6.56337280	−0.59764930	Zn	0.00816990	3.71516020	2.61653680
O	1.67671950	2.87998780	2.10961510	Zn	1.57161130	6.57440300	2.61810850
O	−0.01017210	5.61778100	1.99278190	Zn	1.54149560	2.75992190	5.28304950
O	−0.00226880	3.75597040	4.64706390	O	1.64594820	6.55986390	4.61673390
O	1.60612950	2.80719760	7.29735600	O	1.63336460	8.46485500	1.98951310
Zn	4.87554680	0.92245050	−2.55973590	O	3.25000560	−0.04558880	−3.22822960
O	3.25000040	−1.95090280	−0.65389930	Zn	3.25000180	−0.04781610	0.01857880
O	4.85543390	0.94848980	−0.57233720	Zn	4.87062800	0.99053450	2.60253410
O	3.24999900	0.00353470	2.00956550	O	4.87934150	0.93634360	4.63785780
Zn	3.25000680	3.72162010	−2.61219870	O	4.89439840	2.79842730	−3.20499040
Zn	4.90003550	6.56891180	−2.59880450	O	3.25000120	5.63967880	−3.18279350
Zn	4.83990710	2.82307400	0.14427110	O	3.25000270	3.73818370	−0.62032330
Zn	3.24999060	5.61769680	−0.12848290	O	4.90747040	6.56336630	−0.59763600
O	4.82327400	2.87995570	2.10968050	Zn	4.92831900	6.57433770	2.61808810
O	3.24992800	5.61990830	1.95728020	Zn	4.95857910	2.75988950	5.28313240
O	3.25006440	3.70180120	4.66915050	Zn	3.25000750	5.65364770	5.26000580
O	4.85405490	6.55986550	4.61671960	O	4.89387680	2.80719430	7.29740600
O	3.25000030	5.65061620	7.27111850	O	4.86662810	8.46482150	1.98952000
O	6.52614600	−0.01084220	1.98990720	Zn	6.50715230	3.74366290	−2.56492900
O	6.54820650	5.64379060	−3.23005370	O	6.47760140	3.75752620	−0.57778690
Zn	6.55721580	5.63473000	−0.00281700	O	8.19322890	6.60866390	−0.65415820
Zn	6.49182750	3.71515390	2.61654890	O	8.16470710	2.79579980	1.98591660
O	6.51015540	5.61777530	1.99279410	O	6.50228320	3.75597260	4.64707570

calculated wave numbers in cm^{-1} (unscaled):													
89	93	95	95	96	102	102	106	106	107	108	110	112	113
117	117	119	122	123	125	126	127	128	129	131	132	132	135
138	142	143	144	146	148	148	149	157	158	163	167	167	181
183	185	188	189	195	197	198	199	202	209	210	212	214	215
224	225	230	230	236	237	241	245	248	250	319	324	347	377
381	388	411	413	416	419	420	426	428	429	432	437	438	441
441	443	443	446	447	449	450	451	454	454	455	456	457	458
460	461	462	462	463	464	465	468	469	470	470	472	473	473
475	476	477	477	478	480	481	482	483	485	485	489	490	490
494	494	494	496	497	499	499	505	505	506	507	508	510	511
516	516	520	521	521	522	524	526	527	528	530	530	533	534
534	535	537	538	540	540	542	543	544	544	545	548	550	551
553	553	556	556	557	558	559	561	561	565	573	580	717	831
877	1063	3324	3386										

IR intensities in km/mol:													
2.4	0.4	1.6	0.1	0.2	2.6	0.2	0.3	0.2	0.3	0.3	0.0	0.1	0.0
0.0	0.0	0.4	0.0	0.8	0.2	0.0	0.2	0.0	0.0	0.6	0.1	0.8	0.0
0.7	0.1	0.3	0.3	2.3	1.5	0.6	0.9	0.2	0.2	0.3	1.6	5.4	1.1
1.8	0.2	0.6	0.8	0.0	0.4	0.1	0.0	0.2	1.9	3.3	0.5	0.8	2.1
1.6	0.8	0.2	4.1	6.4	4.0	7.3	9.8	13.4	0.2	16.2	20.7	10.7	21.4
53.4	19.2	0.0	29.4	22.5	19.9	21.6	38.0	162.4	0.1	6.0	0.8	91.2	31.1
0.0	98.6	18.7	12.0	122.4	0.6	44.2	1.6	147.7	102.1	240.5	0.4	2.3	20.8
368.3	13.9	3.6	509.8	115.1	15.9	239.8	5.8	12.5	43.1	2.8	35.6	2.7	94.0
11.0	0.3	64.8	110.7	47.9	62.2	75.6	9.2	32.3	39.7	36.8	27.0	19.8	28.8
164.1	5.2	66.1	113.6	156.5	19.5	32.8	0.7	8.8	583.0	109.8	454.5	129.5	41.8
96.9	1.6	10.1	131.5	38.3	107.5	49.1	72.4	3.8	168.3	7.1	59.2	31.4	35.7
287.4	118.9	318.2	129.6	21.7	165.5	45.8	148.0	37.7	34.4	46.3	90.0	3.4	26.8
48.7	55.4	0.1	127.4	27.2	10.1	66.3	3.5	183.7	133.5	17.6	168.3	1.1	252.4
46.7	58.3	290.2	275.3										

- $2H_{BC_\perp}$-V_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153118.7018912	0.1734378

relaxed coordinates in Å:

H	3.49328310	4.73439790	2.38020140	H	2.51434540	3.05557930	2.39007960
O	−1.68673660	6.60274620	−0.65144170	O	−1.63615230	2.80046740	1.98509890
Zn	1.63153940	0.91188940	−2.58696860	O	1.64670880	0.91835070	−0.59209960
Zn	1.61473890	0.82148800	2.67123700	O	−0.04351740	−0.01845200	1.97810990
O	1.60888750	0.95397290	4.64203990	Zn	−0.01297010	3.75769760	−2.58137830
O	1.60732980	2.80189840	−3.19172250	Zn	1.61371310	6.57555740	−2.58206840
O	−0.04120200	5.65235920	−3.22643730	Zn	1.66005670	2.80566510	−0.04482040
O	0.01448800	3.76480080	−0.57989770	Zn	−0.04106520	5.65263060	0.00325950
O	1.62120390	6.54875410	−0.58069730	Zn	−0.02558970	3.75997150	2.67103250
O	1.63953710	2.76480990	2.01659690	Zn	1.60764300	6.58343980	2.67043610
O	0.02167910	5.61647990	1.99750290	Zn	1.65754250	2.82966720	5.29305870
O	0.00705390	3.73688720	4.64251570	O	1.64253280	6.56861460	4.64206400
O	1.59196620	2.79756730	7.31975720	O	1.63179940	8.45893390	1.98531700
Zn	4.88054900	0.92363760	−2.57770010	O	3.25281510	−0.04984530	−3.23446280
O	3.24785990	−1.95559880	−0.65646390	Zn	3.27018630	−0.05722110	0.00971890
O	4.85556120	0.93875630	−0.59856190	Zn	4.88368270	1.01027350	2.63294060
O	3.25931490	0.00446980	1.99534490	O	4.87856690	0.94774040	4.63894710
Zn	3.26344050	3.74444320	−2.63332060	O	4.89629580	2.80205060	−3.20774010
Zn	4.90122300	6.57435330	−2.58781760	O	3.25196030	5.65013890	−3.19166030
Zn	4.87329480	2.81559570	0.09285490	O	3.26168630	3.74576590	−0.63563320
Zn	3.27531730	5.60386880	−0.04786740	O	4.90374660	6.55864160	−0.59320730
O	4.77036310	2.87532720	2.03853630	Zn	4.97067910	6.63383850	2.67100600
O	3.30202150	5.63915990	2.01333200	Zn	4.83086930	2.83994680	5.23371130
O	3.21953630	3.76929980	4.68152470	Zn	3.25311190	5.59219210	5.29266250
O	4.85290450	6.57288020	4.64179450	O	4.89881250	2.80076420	7.29632790
O	3.24818500	5.66611660	7.31973350	O	4.86914490	8.49007150	1.97817330
O	6.51826930	−0.00866940	1.98451520	Zn	6.51522750	3.75488040	−2.57776370
O	6.54490070	5.65121340	−3.23467370	O	6.48984390	3.76920880	−0.59869220
Zn	6.55971490	5.64007960	0.00975560	O	8.19264370	6.60861070	−0.65637180
Zn	6.44271010	3.70874420	2.63304560	O	8.14199440	2.80282810	1.98435140
O	6.50108090	5.61828800	1.99548220	O	6.49347650	3.74475550	4.63901750

calculated wave numbers in cm^{-1} (unscaled):													
73	85	95	96	96	97	103	103	107	108	110	112	113	115
116	118	118	121	122	125	126	127	127	128	129	131	132	135
136	139	142	143	144	147	148	149	156	157	160	162	165	182
183	183	189	191	196	197	197	199	201	209	211	213	215	215
223	226	229	231	238	239	243	247	248	252	305	318	345	346
363	388	396	396	404	416	423	428	432	433	435	439	440	445
445	447	448	449	450	452	453	455	455	457	458	460	462	463
463	463	466	467	468	468	469	470	472	474	475	475	476	477
478	479	480	480	481	483	483	484	485	485	486	489	491	491
492	495	496	496	501	502	504	505	506	507	508	510	510	512
513	516	517	518	520	520	521	521	523	525	527	527	528	529
532	532	536	536	537	538	539	541	543	544	544	545	545	547
547	548	550	556	557	557	562	567	570	570	586	590	656	788
852	1037	3377	3410										

IR intensities in km/mol:													
1.1	9.7	0.1	0.4	1.1	0.2	0.0	0.0	0.1	0.4	0.0	0.0	0.2	1.5
0.6	0.2	0.6	0.1	0.8	0.4	0.3	1.0	0.9	0.2	3.9	0.5	1.8	0.0
0.1	0.4	0.2	1.2	1.9	1.9	1.5	0.9	0.1	0.6	0.7	3.8	2.1	0.2
1.1	1.7	0.0	0.5	0.0	0.3	0.0	0.5	5.7	2.8	3.0	1.8	1.7	0.1
2.0	0.1	6.2	0.0	6.3	3.6	3.4	12.5	9.7	2.5	13.6	5.6	13.8	13.0
6.0	90.2	32.3	63.3	73.5	0.7	1.3	0.6	13.1	14.5	8.9	2.4	67.7	50.2
228.0	315.1	35.5	71.7	18.4	221.3	28.4	7.7	19.4	1.7	6.0	54.5	134.1	115.0
15.3	18.7	7.2	19.2	74.4	1.7	112.5	38.9	167.4	8.3	24.0	79.9	7.6	7.8
18.2	19.1	30.3	88.4	14.0	93.2	175.9	208.4	21.0	6.7	24.0	89.7	64.1	26.0
5.8	128.9	46.7	41.1	0.7	120.3	232.5	40.9	173.1	16.1	149.5	257.2	127.3	2.9
320.5	34.6	268.5	274.0	149.9	78.2	499.8	113.1	96.7	69.2	103.3	46.6	138.3	19.5
23.3	22.2	1.1	172.9	112.1	392.7	49.8	72.4	50.6	67.8	91.7	29.0	20.5	6.0
5.3	32.7	43.2	47.7	47.0	12.1	0.5	85.8	14.7	5.0	133.6	140.1	0.1	258.9
48.3	59.5	192.1	275.7										

- $3H_{BC_\perp}$-V_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153119.2858636	0.1838396

relaxed coordinates in Å:

H	3.25000010	4.88546810	2.66092020	H	2.26764780	3.18686790	2.66017310
H	4.23236480	3.18686090	2.66016440	O	−1.69565790	6.60791490	−0.65536250
O	−1.66920130	2.78549300	1.97801150	Zn	1.62344000	0.91995190	−2.58039900
O	1.64478730	0.93865890	−0.57662610	Zn	1.59360890	0.82484880	2.67096120
O	−0.04702010	−0.02372880	1.97796330	O	1.62107550	0.95901120	4.64536110
Zn	−0.01649820	3.76032950	−2.58040280	O	1.60874130	2.80506280	−3.18864850
Zn	1.61009240	6.57747390	−2.58027950	O	−0.04144040	5.65286800	−3.22800480
Zn	1.63661720	2.82123020	−0.00311620	O	0.01028460	3.76957550	−0.57660870
Zn	−0.05409370	5.66019130	−0.00659820	O	1.61556060	6.54970600	−0.57648190
Zn	−0.11392720	3.78177780	2.67121820	O	1.57176300	2.78383710	2.07363750
Zn	1.54301350	6.65074290	2.67112850	O	0.00962860	5.62327310	1.99043370
Zn	1.68377520	2.84848760	5.24027850	O	0.01604950	3.73879260	4.64555300
O	1.64501910	6.56021990	4.64556450	O	1.60790880	2.80462690	7.26939500
O	1.62806090	8.49584610	1.97804380	Zn	4.87656000	0.91995200	−2.58039870
O	3.25000000	−0.04781020	−3.22803710	O	3.25000000	−1.95804150	−0.65553160
Zn	3.25000010	−0.06251240	−0.00695030	O	4.85521260	0.93865880	−0.57662610
Zn	4.90639120	0.82484880	2.67096120	O	3.24999980	0.01072620	1.98982920
O	4.87892440	0.95901120	4.64536120	Zn	3.25000010	3.75259800	−2.61794580
O	4.89125870	2.80506280	−3.18864860	Zn	4.88990770	6.57747390	−2.58027950
O	3.25000000	5.64767340	−3.18866980	Zn	4.86338290	2.82123020	−0.00311580
O	3.24999990	3.75275590	−0.59151740	Zn	3.25000000	5.61552440	−0.00264290
O	4.88443940	6.54970600	−0.57648190	O	4.92822300	2.78384520	2.07364970
Zn	4.95698640	6.65074280	2.67112840	O	3.24999990	5.68941170	2.07420710
Zn	4.81622510	2.84848740	5.24027880	O	3.25000060	3.75391420	4.35608990
Zn	3.25000000	5.56206230	5.24103420	O	4.85498090	6.56021990	4.64556440
O	4.89209100	2.80462690	7.26939520	O	3.25000000	5.64877240	7.26995640
O	4.87193910	8.49584610	1.97804380	O	6.54702010	−0.02372890	1.97796340
Zn	6.51649810	3.76032950	−2.58040260	O	6.54144030	5.65286800	−3.22800480
O	6.48971550	3.76957560	−0.57660880	Zn	6.55409370	5.66019120	−0.00659830
O	8.19565800	6.60791510	−0.65536260	Zn	6.61392720	3.78177780	2.67121800
O	8.16920140	2.78549310	1.97801150	O	6.49037140	5.62327330	1.99043360
O	6.48395060	3.73879270	4.64555300				

calculated wave numbers in cm^{-1} (unscaled):													
84	89	92	93	96	96	102	102	107	108	110	110	112	113
113	119	119	124	124	125	126	128	129	129	130	130	132	134
139	139	142	143	147	147	148	150	154	155	160	160	162	182
182	183	187	187	195	196	196	196	199	209	209	211	215	216
226	226	230	232	238	238	241	248	248	253	297	301	322	341
373	374	382	403	407	408	417	417	426	426	430	431	433	434
434	436	443	448	452	452	453	456	456	456	460	461	461	463
463	464	464	465	465	469	469	472	472	473	473	473	474	474
477	477	479	479	480	484	484	485	486	486	486	486	489	489
492	492	493	493	495	495	497	499	499	502	502	505	506	506
506	506	509	512	515	515	515	519	519	520	520	522	524	527
527	528	529	529	530	531	532	533	536	537	537	540	540	541
541	545	549	549	550	550	551	552	552	559	559	559	773	782
791	960	968	971	3316	3320	3366							

IR intensities in km/mol:													
0.0	0.0	1.0	0.0	0.0	0.0	0.2	0.2	0.4	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.2	0.1	1.8	0.0	0.0	0.1	0.0	0.3	0.2	0.0	2.8
0.2	0.2	0.1	0.0	0.5	0.7	0.0	0.1	0.6	0.5	0.1	0.1	0.0	1.4
1.6	0.1	0.0	0.0	0.0	0.3	0.0	0.1	0.8	1.2	1.1	0.0	0.6	0.5
0.9	0.8	3.2	0.0	3.6	3.1	5.9	8.7	9.6	1.2	0.2	0.4	4.3	2.4
9.5	8.0	64.1	0.8	39.7	39.5	0.0	0.0	1.3	1.8	10.7	11.1	0.4	10.6
10.6	3.1	734.7	0.3	13.0	13.2	0.2	86.0	81.9	0.1	0.1	24.2	18.8	0.0
7.0	11.4	13.0	10.5	10.2	103.7	0.0	6.1	7.3	69.8	52.6	0.9	58.9	58.4
3.3	3.7	1.5	128.3	116.2	46.3	19.3	2.8	33.1	56.5	51.7	46.5	3.0	1.0
48.4	47.8	1.1	0.7	105.2	0.2	3.2	32.3	33.5	211.4	227.2	0.5	6.5	0.0
19.3	19.1	0.0	82.4	3.5	2.8	22.0	11.8	37.0	74.2	102.9	39.5	0.1	3.8
8.0	6.0	65.3	72.6	0.5	19.5	25.2	40.0	108.9	24.3	25.8	0.2	1.2	8.8
9.7	0.5	5.8	0.2	0.7	20.2	20.6	0.1	0.5	1.7	6.1	6.3	0.4	0.1
0.4	16.1	2.0	1.1	110.5	110.2	1.2							

- 4H-V_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153119.8427109	0.1917141

relaxed coordinates in Å:

H	3.25000720	4.84148320	2.28776300	H	2.30611440	3.20636700	2.29030390
H	3.24999980	3.74744580	3.80793480	H	4.19388330	3.20635720	2.29031120
O	−1.70253790	6.61188920	−0.65838050	O	−1.67723110	2.78369870	1.97705010
Zn	1.62662890	0.90963970	−2.60237390	O	1.64641360	0.90937550	−0.61177780
Zn	1.59432840	0.83166590	2.64677370	O	−0.05283420	−0.02995960	1.97695170
O	1.62092040	0.94936170	4.63127290	Zn	−0.02382950	3.76823900	−2.60234610
O	1.60405990	2.80236810	−3.19309310	Zn	1.59947970	6.57983760	−2.60248240
O	−0.04832280	5.65675710	−3.24067450	Zn	1.61274930	2.80735310	−0.11226310
O	−0.01412500	3.78554990	−0.61176120	Zn	−0.06030320	5.66376720	−0.01184090
O	1.58932600	6.56291050	−0.61195740	Zn	−0.10718120	3.77894540	2.64709620
O	1.48888510	2.73549900	1.94185120	Zn	1.54889000	6.64619100	2.64685050
O	0.00453650	5.62616230	1.98431560	Zn	1.54310530	2.76709030	5.33939810
O	0.00768610	3.74334020	4.63160410	O	1.63712020	6.56488460	4.63131400
O	1.59892170	2.79948310	7.32915280	O	1.62557620	8.50367050	1.97704510
Zn	4.87336630	0.90963600	−2.60237630	O	3.24999590	−0.05566740	−3.24064760
O	3.25000010	−1.96603100	−0.65858430	Zn	3.25000100	−0.06978740	−0.01227760
O	4.85358700	0.90937640	−0.61177970	Zn	4.90567080	0.83166050	2.64677370
O	3.24999840	0.00489190	1.98376310	O	4.87907970	0.94935950	4.63127280
Zn	3.25000400	3.75242300	−2.65092470	O	4.89594490	2.80236500	−3.19309540
Zn	4.90051620	6.57983920	−2.60248320	O	3.24999870	5.65294720	−3.19303320
Zn	4.88724970	2.80735400	−0.11226250	O	3.24999950	3.75236770	−0.62892900
Zn	3.25000120	5.64303870	−0.11313470	O	4.91067530	6.56291080	−0.61195900
O	5.01111530	2.73549300	1.94185180	Zn	4.95110990	6.64618970	2.64685340
O	3.25000020	5.78503270	1.94089030	Zn	4.95689580	2.76708610	5.33940280
O	3.25000190	3.75150280	4.82227500	Zn	3.24999640	5.72235100	5.33872860
O	4.86287600	6.56488240	4.63131700	O	4.90107800	2.79948290	7.32915740
O	3.24999960	5.65912190	7.32881670	O	4.87442380	8.50366870	1.97704600
O	6.55283500	−0.02996060	1.97695130	Zn	6.52383070	3.76824150	−2.60234760
O	6.54832050	5.65676050	−3.24067440	O	6.51412430	3.78554970	−0.61176250
Zn	6.56030600	5.66376820	−0.01184590	O	8.20254100	6.61189090	−0.65838200
Zn	6.60717660	3.77894740	2.64709740	O	8.17722790	2.78370050	1.97705150
O	6.49546300	5.62616350	1.98431190	O	6.49231230	3.74333950	4.63160630

calculated wave numbers in cm^{-1} (unscaled):													
89	89	91	93	98	98	102	102	107	107	108	109	111	112
115	115	116	121	122	122	124	124	126	128	128	129	131	133
135	137	142	143	146	146	147	155	156	156	159	161	161	185
185	187	190	190	196	197	198	200	200	210	210	212	218	218
226	226	231	235	241	241	244	251	251	251	303	304	306	320
397	398	400	418	421	423	424	426	430	433	434	442	442	443
449	450	453	456	456	456	456	456	458	460	460	461	462	465
466	466	469	470	470	471	472	473	473	476	476	479	479	480
481	481	482	483	484	484	484	485	487	487	489	490	490	494
495	496	496	497	497	500	501	501	501	504	505	506	506	506
508	511	511	518	519	519	519	520	522	522	525	526	526	530
531	534	536	537	537	539	539	540	541	545	545	546	546	547
550	552	552	552	555	555	555	561	561	564	573	573	696	700
736	752	764	794	849	915	2788	2998	3065	3072				

IR intensities in km/mol:													
0.0	0.0	0.8	0.0	0.1	0.0	0.3	0.2	0.2	0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.0	0.1	0.1	0.3	0.3	0.2	0.0	0.2	0.0	0.3	0.0	3.1
0.1	0.1	0.0	0.0	0.8	0.9	0.1	0.2	0.3	0.1	0.1	0.0	0.2	1.6
1.6	0.0	0.0	0.0	1.0	0.6	0.1	0.0	0.0	1.3	1.3	0.2	0.0	0.0
0.6	0.7	1.9	0.0	5.0	4.2	4.3	9.9	11.8	6.3	8.6	10.4	9.1	0.2
2.3	3.7	133.4	3.2	1.0	67.3	0.2	61.3	0.5	1.2	1.9	0.2	0.3	0.0
1.1	1.0	404.7	2.6	5.0	66.3	45.9	19.0	94.2	0.1	45.1	41.5	0.0	4.2
20.1	23.0	9.4	9.4	9.6	0.1	379.3	13.4	12.8	0.4	0.8	48.7	43.0	0.3
24.8	21.9	79.3	49.4	57.8	5.2	5.2	82.0	66.6	74.3	0.0	87.8	78.6	3.6
10.1	4.5	7.9	87.3	79.4	53.6	97.9	97.0	0.0	123.2	147.7	155.5	5.7	13.8
0.4	9.8	11.4	49.4	0.0	125.2	131.5	52.4	11.1	10.5	86.5	93.2	86.5	9.8
10.0	0.0	99.5	109.3	80.0	29.8	25.5	14.3	0.5	1.0	0.4	13.9	12.9	0.0
0.3	5.2	4.7	0.0	3.0	3.5	8.1	13.8	13.8	0.1	18.1	18.2	24.4	29.2
63.2	0.3	41.8	40.5	2.3	0.6	426.6	335.9	462.1	457.9				

2.3 Hydrogen at Substitutional Copper Atoms

- $H_{BC_\perp}$-Cu_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-154758.4406579	0.1637360

relaxed coordinates in Å:

H	3.97886540	3.33298840	−0.43790710	O	−1.69291500	6.60631890	−0.65496270
O	−1.66155590	2.79269330	1.98022820	Zn	1.63116520	0.90907350	−2.58479490
O	1.64345600	0.92636950	−0.59491100	Zn	1.60436310	0.92113750	2.64319920
O	−0.03703830	−0.01629800	1.98174940	O	1.61597640	0.95435860	4.64219790
Zn	−0.02246060	3.76369160	−2.58233520	O	1.59034300	2.79727690	−3.19947850
Zn	1.60408140	6.58093840	−2.58255120	O	−0.04311140	5.65371700	−3.23222460
Zn	1.56722520	2.77378210	0.05700060	O	0.00009930	3.77984560	−0.59350820
Zn	−0.05246540	5.65932350	0.01438890	O	1.60130670	6.55370480	−0.59390510
Zn	−0.03531350	3.74663080	2.64384740	O	1.60983760	2.81728370	2.03433350
Zn	1.61245740	6.60076480	2.64400960	O	0.00728420	5.62479240	2.00266780
Zn	1.60644430	2.80547430	5.30717160	O	0.00525730	3.74224810	4.64102200
O	1.63671670	6.56773420	4.64114060	O	1.59745240	2.80049280	7.31984850
O	1.62561590	8.48596910	1.98019670	Zn	4.87697780	0.92732410	−2.57690590
O	3.24814490	−0.04984830	−3.23857840	O	3.24480530	−1.96304330	−0.65578710
Zn	3.25329290	−0.06110620	0.01529950	O	4.83717610	0.87413700	−0.62033310
Zn	4.88825300	0.89591680	2.65628240	O	3.23869020	0.00613710	2.00673600
O	4.87825720	0.93874710	4.66381230	Zn	3.23727890	3.75997870	−2.73801710
O	4.88201160	2.81060950	−3.20518580	Zn	4.90326250	6.57621340	−2.58496580
O	3.24752370	5.66756860	−3.19953530	Cu	5.44786060	2.48310060	0.39920770
O	3.13685250	3.81849470	−0.68161660	Zn	3.25612000	5.70009630	0.05686170
O	4.89426610	6.55730780	−0.59522070	Zn	3.22412280	3.76784070	2.71162990
O	4.86362290	2.82156790	2.25105230	Zn	4.87925550	6.59360420	2.64342350
O	3.23986440	5.64107090	2.03417220	Zn	4.88311940	2.80979900	5.26948820
O	3.22871300	3.76494230	4.72344400	Zn	3.24851720	5.64952600	5.30752370
O	4.85631090	6.56676270	4.64230230	O	4.89650340	2.80211440	7.30310930
O	3.24839230	5.65999410	7.32022250	O	4.87057550	8.48361790	1.98170140
O	6.53818370	−0.02363630	1.98855370	Zn	6.51049840	3.75640990	−2.57648000
O	6.54237630	5.65548630	−3.23860390	O	6.53631320	3.81768550	−0.61977640
Zn	6.55428350	5.65701150	0.01540460	O	8.19745730	6.61496440	−0.65562670
Zn	6.54356420	3.76262550	2.65645560	O	8.16444980	2.79323730	1.98852550
O	6.48881960	5.63594260	2.00688450	O	6.50113450	3.74952860	4.66391450

calculated wave numbers in cm^{-1} (unscaled):													
30	56	88	93	94	94	97	97	100	105	108	108	110	111
112	113	115	118	120	120	121	125	129	130	132	133	134	135
137	140	141	141	142	143	144	149	150	155	156	159	176	183
184	185	185	189	192	196	197	198	199	206	210	213	214	215
220	221	229	231	232	235	238	243	244	247	248	255	255	360
371	381	401	406	413	422	425	433	433	436	440	440	445	446
448	448	449	451	451	452	453	455	456	456	458	460	461	463
463	464	464	464	468	468	468	469	469	471	472	472	474	477
478	478	479	479	481	482	486	486	487	488	488	488	491	492
493	494	495	495	497	498	500	501	503	505	506	509	510	511
513	515	516	519	520	523	524	526	526	527	528	531	531	532
535	535	537	537	539	540	541	542	543	543	544	545	545	547
548	550	550	551	551	553	556	557	560	560	562	568	575	578
587	686	693	3180										

IR intensities in km/mol:													
0.9	0.4	0.4	0.1	0.2	0.0	0.0	0.2	0.1	0.5	0.2	0.1	0.1	0.1
0.1	0.0	0.0	0.1	0.1	0.7	0.1	0.1	0.1	0.1	0.1	0.0	0.1	0.1
0.3	0.3	0.4	0.0	0.3	0.4	0.2	1.6	1.7	0.1	0.0	0.2	0.4	2.8
3.3	1.2	0.1	0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.5	0.4	0.3	2.2
1.8	1.5	0.8	0.4	0.8	0.2	4.3	3.3	5.1	0.7	3.3	9.5	4.8	21.0
52.4	40.3	64.0	80.2	39.6	1.6	0.0	61.3	0.1	1.0	0.0	0.2	70.9	18.2
144.4	2.4	93.4	40.6	77.7	18.7	142.8	15.2	0.6	2.2	0.4	23.6	676.2	33.1
14.4	84.8	4.2	4.1	109.3	89.4	9.7	124.5	185.1	54.2	18.6	2.5	60.6	31.2
0.7	2.5	16.8	111.0	111.8	11.1	2.0	102.1	7.3	152.8	34.6	20.1	0.4	33.0
134.8	83.5	291.3	22.6	69.2	39.3	7.8	9.6	52.1	249.8	23.4	366.9	600.9	24.0
299.7	11.9	11.5	88.5	109.9	3.9	77.6	94.4	56.9	172.9	135.2	37.9	12.4	175.4
74.2	64.4	72.9	198.0	26.9	206.4	9.0	100.1	70.9	364.7	3.2	131.2	54.2	50.6
16.2	8.9	47.5	77.8	11.5	5.5	2.2	64.5	42.7	30.3	11.2	8.2	148.9	159.1
62.1	76.2	74.9	531.6										

- $H_{BC_{\parallel}}$-Cu_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-154758.4392301	0.1640879

relaxed coordinates in Å:

H	4.69941190	2.91864060	1.20327140	O	−1.68855970	6.60380740	−0.65114850
O	−1.67105260	2.78724460	1.98250690	Zn	1.61901750	0.93123270	−2.58006710
O	1.62443680	0.93469710	−0.58842310	Zn	1.58420350	0.92469160	2.64174550
O	−0.04147880	−0.02262130	1.98528930	O	1.62065830	0.95325230	4.64716940
Zn	−0.00853900	3.75766120	−2.57458480	O	1.62052750	2.81293910	−3.18976930
Zn	1.61626140	6.57193410	−2.57452540	O	−0.04148650	5.65283910	−3.22799730
Zn	1.67845380	2.82310780	0.02449230	O	0.01589970	3.76176750	−0.57952900
Zn	−0.03544520	5.64938530	−0.00154740	O	1.62499840	6.54876150	−0.57950420
Zn	−0.05072010	3.74695620	2.62495570	O	1.59883260	2.80985410	2.04285440
Zn	1.60445610	6.61380370	2.62497080	O	0.00539930	5.62578300	1.99999270
Zn	1.59231890	2.80221810	5.31030380	O	0.00622290	3.74304600	4.63515770
O	1.63650200	6.56650230	4.63517340	O	1.60020980	2.80007060	7.32220540
O	1.62557920	8.49683330	1.98248160	Zn	4.85781670	0.89643500	−2.61975450
O	3.22520660	−0.05833970	−3.24394380	O	3.24294750	−1.98013190	−0.65606340
Zn	3.18841620	−0.08647590	0.01765200	O	4.80334210	0.75308520	−0.63286170
Zn	4.88252920	0.85687990	2.64811950	O	3.22967840	0.01129120	2.01327730
O	4.88143000	0.95719800	4.63962460	Zn	3.25819860	3.74784470	−2.54614470
O	4.89235880	2.80457640	−3.20880780	Zn	4.87791810	6.57564040	−2.58020160
O	3.24897240	5.63353930	−3.18976240	Cu	5.20075440	2.62665120	−0.59597610
O	3.32172830	3.71127650	−0.54760720	Zn	3.26923720	5.57843530	0.02444180
O	4.87761050	6.56944450	−0.58865220	Zn	3.11218140	3.83210520	2.76273980
O	4.82067730	2.84658050	2.19981650	Zn	4.86603570	6.60912190	2.64197640
O	3.24081270	5.65381110	2.04292420	Zn	4.88052200	2.81119010	5.30146260
O	3.23478950	3.76132750	4.74505120	Zn	3.24425510	5.66331380	5.31054580
O	4.85959420	6.56326060	4.64724270	O	4.89991850	2.80012720	7.31389070
O	3.25012780	5.65781580	7.32250420	O	4.87385030	8.49051570	1.98524490
O	6.53278420	−0.01351330	1.98945540	Zn	6.52766790	3.78842010	−2.61927810
O	6.53818460	5.67956200	−3.24392020	O	6.62460020	3.90746130	−0.63218490
Zn	6.54393260	5.72584530	0.01780190	O	8.21129300	6.62513840	−0.65590260
Zn	6.57469030	3.78714040	2.64879220	O	8.15306710	2.79285520	1.98956030
O	6.47978300	5.64098370	2.01344820	O	6.48666990	3.73750790	4.64003230

calculated wave numbers in cm^{-1} (unscaled):													
46	85	88	93	94	96	98	101	105	107	108	109	110	111
112	113	116	118	120	121	124	127	129	131	133	135	135	136
137	142	142	143	145	145	146	150	151	156	157	158	174	182
184	185	185	191	194	196	198	198	201	204	207	208	211	215
218	223	223	228	232	232	236	237	242	245	246	249	254	341
353	406	410	415	417	417	425	433	434	436	437	442	443	443
446	447	451	451	452	453	453	455	456	457	457	460	461	461
461	463	465	466	467	467	468	469	470	470	471	472	473	475
475	477	478	479	481	482	483	483	484	486	487	488	489	491
492	493	494	494	496	498	498	500	502	504	505	506	508	510
511	512	514	516	517	518	519	520	523	525	527	528	529	530
530	531	532	535	538	539	540	540	542	543	544	546	548	549
549	551	552	553	554	555	557	558	559	562	565	576	578	613
617	760	799	3111										

IR intensities in km/mol:													
0.3	0.3	0.7	0.1	0.2	0.1	0.1	0.4	0.2	0.1	0.1	0.0	0.1	0.1
0.0	0.0	0.5	0.0	0.2	0.9	0.4	0.2	0.1	0.1	0.0	0.1	0.0	0.0
0.1	0.5	0.4	0.3	0.6	0.6	0.1	0.7	0.7	0.0	0.0	0.1	0.0	2.7
2.0	0.5	0.3	0.1	0.4	0.5	0.1	0.0	1.0	1.6	2.0	3.4	0.8	1.3
0.1	0.6	0.3	7.0	1.8	2.5	1.1	8.2	3.5	4.5	5.5	2.9	5.9	17.6
38.4	29.1	78.5	14.5	28.2	6.9	159.0	0.7	2.3	98.6	0.8	92.3	20.8	8.2
5.8	25.7	11.2	22.9	1.0	64.9	52.6	6.2	128.8	7.6	71.6	183.9	75.8	18.6
14.4	28.1	372.0	29.4	3.4	178.3	1.0	131.9	24.4	202.3	20.9	19.6	19.1	102.4
9.9	84.3	9.8	40.4	48.7	10.4	51.2	70.3	42.7	104.9	22.1	209.9	165.4	78.3
53.9	78.0	59.2	158.5	0.2	42.3	106.5	7.7	18.7	185.5	44.0	125.7	273.2	350.0
166.6	235.4	16.1	315.9	150.5	36.8	38.0	136.1	134.4	288.6	5.1	95.1	226.1	99.5
8.2	36.6	5.9	1.8	127.6	5.7	17.5	58.6	3.4	17.7	59.0	197.2	53.8	57.1
7.3	18.3	21.7	91.8	1.3	76.3	7.1	9.7	15.9	134.8	33.7	135.9	142.4	175.0
8.7	44.7	69.0	525.2										

- $H_{AB_{\parallel}}$-Cu_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-154758.4142216	0.1646508

relaxed coordinates in Å:

H	4.87668020	2.80498650	3.38285020	O	−1.69271840	6.60620960	−0.65132940
O	−1.67590380	2.78528620	1.98301640	Zn	1.62637980	0.92921400	−2.59497130
O	1.61658170	0.93156230	−0.60173740	Zn	1.57194570	0.92556640	2.64246850
O	−0.04669430	−0.02558410	1.98506900	O	1.62228720	0.95299020	4.64707830
Zn	−0.00689920	3.75840440	−2.58073110	O	1.62146130	2.81352230	−3.19164770
Zn	1.61647750	6.57012960	−2.58073020	O	−0.04341580	5.65394730	−3.23005590
Zn	1.66649870	2.82099790	−0.00596610	O	0.00398600	3.76790780	−0.58580020
Zn	−0.03967840	5.65189150	−0.00553280	O	1.61376510	6.55601680	−0.58586500
Zn	−0.06312600	3.75040630	2.62407760	O	1.56917380	2.79915090	2.01863990
Zn	1.59544600	6.62286070	2.62410540	O	0.00480430	5.62620990	1.99929540
Zn	1.61614760	2.81361240	5.28250710	O	0.01117850	3.74214840	4.63507250
O	1.63980860	6.56259710	4.63509400	O	1.60631670	2.80143830	7.30494750
O	1.62483880	8.50203050	1.98296120	Zn	4.87093220	0.92001710	−2.57658860
O	3.24422600	−0.05352830	−3.23590230	O	3.24274480	−1.98730230	−0.65732820
Zn	3.17499220	−0.09158370	−0.00339490	O	4.79949980	0.76484750	−0.59178920
Zn	4.87725380	0.77672250	2.58026510	O	3.20074420	−0.00262630	1.99977780
O	4.88229880	0.97083630	4.62282970	Zn	3.26949950	3.74130650	−2.54647310
O	4.89505530	2.80290350	−3.21013410	Zn	4.88346950	6.57031170	−2.59495120
O	3.24902750	5.63243160	−3.19159630	Cu	5.16702310	2.64645630	−0.37593950
O	3.30054870	3.72362570	−0.55559680	Zn	3.26531310	5.59003770	−0.00616370
O	4.87680460	6.57778030	−0.60183980	Zn	3.08796490	3.84650970	2.62408460
O	4.86093870	2.82081600	2.39551010	Zn	4.85979590	6.61906640	2.64247920
O	3.23543940	5.68517830	2.01837150	Zn	4.88782610	2.80747480	5.39251870
O	3.27136440	3.73998640	4.67271270	Zn	3.24640430	5.63682240	5.28259500
O	4.86066490	6.56198620	4.64708430	O	4.90080320	2.79956850	7.35858400
O	3.25196930	5.65177420	7.30513990	O	4.87384350	8.49639930	1.98503660
O	6.55467120	−0.03025970	1.98576740	Zn	6.51369030	3.76532350	−2.57678110
O	6.54354090	5.66081950	−3.23603360	O	6.61301630	3.90491150	−0.59228420
Zn	6.54189940	5.73950680	−0.00269990	O	8.21736820	6.62891230	−0.65712310
Zn	6.63780970	3.82954590	2.58227930	O	8.17731010	2.78265800	1.98622860
O	6.47752330	5.67144290	2.00033320	O	6.47524180	3.72973600	4.62386850

calculated wave numbers in cm^{-1} (unscaled):													
76	79	87	87	90	95	96	97	98	99	102	105	105	108
109	111	112	117	117	121	123	124	128	129	130	132	135	135
136	137	141	143	144	144	145	149	150	154	155	158	161	172
182	184	184	189	191	193	196	197	205	207	207	210	210	215
216	222	224	225	232	233	234	235	240	244	245	247	255	304
362	381	387	413	417	418	425	428	429	435	435	441	442	443
445	447	448	449	451	451	452	454	454	456	457	460	460	461
461	464	464	465	465	466	468	469	470	472	473	474	474	475
476	477	479	480	481	481	483	485	485	486	488	491	491	492
494	497	499	499	499	501	501	503	505	507	507	509	510	511
512	515	515	516	517	519	519	522	523	524	526	528	529	531
532	533	534	536	537	538	541	543	544	545	546	546	547	548
552	555	556	557	558	559	560	561	562	569	572	573	583	601
610	770	792	3480										

IR intensities in km/mol:													
0.0	0.2	0.4	0.5	0.4	0.2	0.1	0.0	0.5	0.1	0.9	0.1	0.3	0.1
0.1	0.2	0.0	0.0	0.1	1.2	0.5	0.5	0.0	0.3	0.6	0.3	0.0	0.0
0.1	0.4	1.1	0.1	0.1	0.5	0.4	1.2	0.3	0.3	0.2	0.1	0.3	7.4
2.8	1.6	1.1	0.1	0.0	2.5	0.3	0.0	2.9	2.3	2.2	1.9	0.8	0.9
0.7	3.4	0.6	1.6	3.0	3.3	0.7	10.0	3.5	7.3	4.1	2.7	1.9	19.9
24.4	30.8	21.5	1.3	20.3	18.9	290.1	29.0	1.2	10.8	1.5	4.2	63.3	12.8
64.8	92.0	3.9	69.0	23.8	430.1	8.5	55.1	60.7	0.4	82.6	0.9	10.8	58.2
59.6	82.5	2.1	11.0	22.5	4.4	5.8	30.0	6.1	255.8	4.1	14.9	73.3	334.9
6.3	13.0	4.7	74.5	138.0	4.4	103.0	160.5	42.4	308.2	3.3	61.0	58.2	5.7
208.9	1.8	125.2	43.4	42.1	25.1	23.9	60.6	100.0	28.9	429.7	76.4	24.8	16.1
376.9	217.4	19.0	119.1	11.7	84.8	273.8	26.2	125.6	218.1	113.0	104.2	35.0	109.6
40.9	43.7	25.9	149.0	84.3	44.4	31.6	16.9	8.8	30.2	97.3	19.8	135.0	76.3
8.3	6.9	6.4	11.9	0.1	2.5	49.4	3.8	55.3	155.1	73.2	110.4	116.1	183.0
2.2	95.2	82.8	39.6										

- $H_{AB_{\perp}}$-Cu_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-154758.4236752	0.1654905

relaxed coordinates in Å:

H	1.96569820	4.49363500	−1.03859230	O	−1.69096310	6.60521850	−0.65426700
O	−1.65766350	2.79500060	1.97979340	Zn	1.63533740	0.91074260	−2.59554510
O	1.64115840	0.90021800	−0.60619440	Zn	1.60314630	0.90530110	2.67898230
O	−0.03557690	−0.01415720	1.98171160	O	1.61318770	0.95573370	4.66619080
Zn	−0.01821090	3.75070570	−2.58919700	O	1.60753600	2.79969830	−3.20222010
Zn	1.61746980	6.58373000	−2.58918910	O	−0.03774050	5.65064780	−3.22517430
Zn	1.55567530	2.68714720	0.13544420	O	0.01128550	3.77330950	−0.58814690
Zn	−0.05806400	5.66278530	0.02853010	O	1.61315340	6.54699980	−0.58839720
Zn	−0.03344780	3.74741790	2.65913120	O	1.61362260	2.80601290	2.08074710
Zn	1.61293230	6.59859970	2.65919490	O	0.00922070	5.62371870	2.01023730
Zn	1.62114200	2.81481450	5.30348170	O	0.00672850	3.74196480	4.65094410
O	1.63772250	6.56658740	4.65100930	O	1.59912710	2.80197460	7.31817350
O	1.62556780	8.48139650	1.97978680	Zn	4.87754610	0.90462820	−2.56612220
O	3.24727480	−0.05341140	−3.24362690	O	3.24114980	−1.98407380	−0.66137860
Zn	3.21432710	−0.10893000	0.05062410	O	4.79012710	0.78246960	−0.61316340
Zn	4.89998730	0.94678200	2.60558410	O	3.23265360	0.00813220	2.02699210
O	4.87752630	0.94371400	4.62991870	Zn	3.29676650	3.72551980	−2.74373800
O	4.91959770	2.78885540	−3.20520510	Zn	4.90387520	6.57177610	−2.59558140
O	3.25403250	5.65142710	−3.20215310	Cu	5.32494960	2.55541320	−0.08203510
O	2.79166220	4.01674460	−0.77178480	Zn	3.32557180	5.75210040	0.13512990
O	4.91557030	6.57202460	−0.60637840	Zn	3.28890190	3.73017420	2.68000570
O	4.87230150	2.81600850	2.01376290	Zn	4.89233510	6.60227620	2.67891930
O	3.25152940	5.64292020	2.08038760	Zn	4.89713420	2.80175130	5.27455040
O	3.24777900	3.75395660	4.69945050	Zn	3.24784130	5.63217050	5.30377500
O	4.85379210	6.56851240	4.66612950	O	4.89800220	2.80125960	7.30340460
O	3.24794960	5.65780660	7.31851550	O	4.86945660	8.48118600	1.98166850
O	6.53891420	−0.02503940	1.98423610	Zn	6.53036420	3.76728080	−2.56604150
O	6.54499760	5.65814680	−3.24368770	O	6.59336290	3.90449900	−0.61312660
Zn	6.57632350	5.71476220	0.05061270	O	8.21385990	6.62871690	−0.66123590
Zn	6.50505350	3.72673080	2.60556150	O	8.16614360	2.79335260	1.98423350
O	6.48413580	5.63990170	2.02691410	O	6.49644810	3.74770040	4.62985530

calculated wave numbers in cm^{-1} (unscaled):													
66	90	91	92	94	96	98	98	100	104	106	107	108	110
112	113	113	116	118	120	123	125	127	129	130	132	134	135
137	138	140	141	142	142	143	149	151	155	157	159	178	180
183	185	185	191	193	196	196	198	199	209	209	211	212	216
217	220	225	229	230	233	239	239	244	245	248	250	253	277
347	410	415	417	422	422	425	427	431	431	440	441	443	445
446	450	452	453	453	454	455	456	457	458	458	459	462	462
463	465	465	465	467	469	469	469	470	470	472	475	475	477
478	479	480	481	481	483	484	484	486	489	489	490	490	491
494	494	497	498	499	500	501	504	506	508	509	510	512	514
515	516	518	519	521	522	524	526	527	529	529	530	531	531
533	534	536	537	537	539	540	540	542	543	546	546	547	549
550	551	552	554	554	555	557	559	561	567	569	574	577	601
611	871	910	3441										

IR intensities in km/mol:													
0.2	0.3	0.0	0.7	0.1	0.7	0.0	0.1	0.2	0.3	0.4	0.1	0.0	0.3
0.1	0.0	0.1	0.1	0.1	0.1	0.6	0.1	0.0	0.0	0.1	0.1	0.1	0.1
0.0	0.7	0.0	0.1	0.0	0.1	0.3	1.1	1.6	0.0	0.0	0.4	1.1	0.3
1.9	1.5	0.9	2.2	0.1	0.7	1.0	1.0	0.5	3.3	1.5	1.1	1.7	1.1
1.0	2.5	2.5	0.2	0.5	1.5	1.8	1.6	10.9	2.3	2.4	16.4	13.5	4.6
44.3	57.2	20.6	19.3	9.9	18.3	3.0	65.3	9.2	2.3	35.8	7.0	84.4	11.1
38.8	0.2	75.9	13.8	127.3	147.5	0.3	26.9	99.5	23.1	13.1	84.5	516.1	151.6
14.8	42.1	145.2	126.3	39.2	66.9	7.0	58.4	71.4	9.0	72.3	65.4	54.6	60.3
1.0	8.3	6.2	63.8	66.2	58.5	13.5	54.9	64.2	165.6	55.7	39.5	1.5	106.1
130.3	69.7	0.7	182.4	32.7	74.2	27.7	97.2	292.6	3.7	81.1	49.9	612.4	65.6
120.8	196.6	184.1	51.0	108.4	161.3	118.3	29.8	92.9	40.4	72.8	0.2	114.9	213.5
2.3	2.5	104.3	12.2	203.9	19.0	10.4	38.7	79.7	26.4	4.8	170.2	127.2	18.9
106.8	4.0	48.2	24.6	16.0	40.0	62.6	15.3	2.5	42.0	51.0	115.7	143.1	167.9
0.7	107.8	57.3	44.5										

- $H_{BC_\perp}$-$H_{BC_\parallel}$-Cu_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-154759.0082419	0.1745804

relaxed coordinates in Å:

H	3.92701540	3.36215190	−0.37729910	H	4.85400410	2.82952730	1.19849260
O	−1.70139420	6.61124560	−0.65859980	O	−1.66404510	2.78917740	1.97929740
Zn	1.60850770	0.92326060	−2.58365730	O	1.63405100	0.94045370	−0.59808690
Zn	1.58381370	0.91999010	2.66287370	O	−0.03685880	−0.02004560	1.97999410
O	1.62054980	0.95491570	4.65435870	Zn	−0.02995640	3.77130350	−2.58664550
O	1.59185970	2.80309850	−3.20004790	Zn	1.59378470	6.58362340	−2.58686510
O	−0.04610100	5.65548430	−3.23886660	Zn	1.51939900	2.78078490	0.07053350
O	−0.01589140	3.79279130	−0.60136360	Zn	−0.06812930	5.66854420	0.01786850
O	1.58251390	6.56098620	−0.60177540	Zn	−0.05309370	3.74997680	2.65069110
O	1.60571670	2.81078170	2.04484060	Zn	1.60095480	6.61432910	2.65068490
O	0.01028160	5.62313720	2.00468020	Zn	1.59802850	2.80395680	5.32355920
O	0.00912830	3.74055050	4.64574510	O	1.64014940	6.56521390	4.64573750
O	1.60019650	2.79995510	7.32954750	O	1.62745150	8.48981200	1.97925030
Zn	4.83750530	0.87788480	−2.66840770	O	3.21056450	−0.06287820	−3.25297340
O	3.24520490	−1.97312480	−0.65948220	Zn	3.17302890	−0.09910190	0.04194440
O	4.78307310	0.75056190	−0.66469890	Zn	4.88949060	0.83770180	2.68537210
O	3.23554080	0.01750560	2.01660860	O	4.88327540	0.95888550	4.65749070
Zn	3.21965030	3.77007510	−2.71460800	O	4.88221090	2.81043170	−3.18534780
Zn	4.87960330	6.58871980	−2.58404680	O	3.24321830	5.66322160	−3.20007270
Cu	5.59144970	2.40129460	−0.59535060	O	3.09645820	3.84152260	−0.64485900
Zn	3.22653900	5.73758880	0.07016970	O	4.87754150	6.55841820	−0.59868810
Zn	3.13258730	3.82059000	2.76977440	O	4.84750130	2.83079610	2.19564690
Zn	4.87000430	6.61191340	2.66314150	O	3.24378710	5.64756310	2.04445060
Zn	4.87863650	2.81226810	5.32377480	O	3.24066760	3.75806340	4.74156920
Zn	3.24560590	5.65759500	5.32396170	O	4.85809850	6.56252600	4.65444860
O	4.90014290	2.80000360	7.32735700	O	3.25022330	5.65793160	7.32995670
O	4.87393230	8.48527500	1.97991570	O	6.53440400	−0.01440630	1.97810090
Zn	6.53343750	3.81532690	−2.66861320	O	6.53486270	5.69462420	−3.25306930
O	6.61703750	3.92650090	−0.66495650	Zn	6.54712760	5.74544600	0.04195160
O	8.20627570	6.61964270	−0.65934820	Zn	6.59458890	3.79053300	2.68596540
O	8.15470980	2.79187830	1.97818560	O	6.47723900	5.63273170	2.01670090
O	6.48610000	3.73504000	4.65782680				

calculated wave numbers in cm^{-1} (unscaled):													
82	87	90	92	93	96	97	99	101	105	107	108	109	110
112	114	115	117	118	121	122	125	128	129	131	133	133	134
136	139	141	141	143	143	145	149	150	156	156	159	169	177
185	186	188	192	192	196	197	198	201	201	209	211	212	218
221	225	225	230	231	237	238	240	246	247	249	253	257	329
350	397	398	399	400	411	419	423	424	430	436	438	443	443
444	446	447	452	453	454	456	457	457	459	459	460	462	463
463	465	466	466	467	468	468	469	470	471	471	474	475	477
478	478	479	480	481	483	484	484	485	485	485	486	489	490
492	492	494	494	495	497	499	500	502	503	504	505	508	508
508	509	510	510	514	516	517	517	520	521	522	523	526	526
530	530	531	532	532	535	535	536	538	538	540	541	544	545
547	548	549	551	552	552	554	555	559	560	563	576	577	614
647	667	693	709	859	3248	3270							

IR intensities in km/mol:													
0.1	0.2	0.1	0.0	0.1	0.1	0.1	0.5	0.4	0.1	0.0	0.1	0.3	0.1
0.1	0.0	0.2	0.0	0.0	0.3	0.2	0.3	0.0	0.0	0.8	0.0	0.1	0.0
0.0	0.1	0.5	0.1	0.6	0.0	0.3	0.6	0.4	0.0	0.0	0.1	0.2	0.2
2.5	0.1	1.2	0.2	0.3	0.0	0.0	0.0	0.1	0.2	0.5	1.4	0.3	0.0
0.0	0.2	0.1	2.1	0.9	0.4	0.8	6.7	5.0	4.9	4.8	6.0	9.7	13.5
1.0	10.1	8.2	31.7	91.2	26.4	1.5	13.2	0.8	0.5	21.5	0.5	4.5	11.0
15.4	4.1	38.6	320.3	4.8	2.3	77.8	106.2	15.7	148.2	67.3	186.5	22.2	7.2
17.9	35.9	10.8	6.0	34.0	43.4	33.6	6.8	9.4	35.7	11.5	2.4	198.0	30.6
94.0	34.1	73.0	0.1	46.9	146.8	15.6	14.4	23.3	5.2	70.1	72.4	88.7	49.2
17.1	9.2	13.2	27.8	20.8	0.4	19.1	13.5	23.4	96.1	116.2	31.7	36.9	2.0
11.5	9.1	41.6	76.2	22.8	37.4	78.9	2.5	62.8	5.5	2.0	29.6	5.1	3.6
12.6	20.8	6.7	2.2	5.5	8.7	3.4	0.7	143.5	29.6	12.7	21.2	18.7	11.6
15.6	20.6	2.7	0.5	26.1	1.4	9.2	23.8	7.2	4.8	6.8	29.5	32.7	0.5
3.9	1.7	21.4	0.6	8.6	106.6	50.2							

- $2H_{BC_\perp}$-Cu_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-154759.0052501	0.1742515

relaxed coordinates in Å:

calculated wave numbers in cm^{-1} (unscaled):													
71	81	86	91	92	93	95	96	99	105	107	109	110	111
111	114	115	117	118	120	122	124	127	128	129	131	133	134
138	139	140	140	141	142	147	149	153	155	158	159	167	180
184	186	187	191	192	195	198	199	200	204	211	212	215	217
221	226	228	229	232	237	240	244	246	247	249	255	257	327
349	355	398	409	409	411	423	429	432	437	438	440	442	445
446	446	447	450	451	452	454	455	456	457	459	459	461	463
464	465	465	466	467	468	468	470	471	471	472	474	475	476
477	478	480	481	482	484	485	485	486	487	487	489	490	491
491	492	493	496	497	497	498	500	500	503	504	506	508	508
509	511	512	515	516	517	518	520	520	521	525	526	527	529
530	531	533	533	534	536	536	538	539	540	542	543	543	546
548	549	550	550	552	553	555	557	559	562	565	577	578	580
618	630	679	697	840	3220	3252							

IR intensities in km/mol:													
0.5	1.0	0.3	0.0	0.1	0.0	0.1	0.1	0.4	0.1	0.0	0.0	0.2	0.1
0.1	0.0	0.1	0.0	0.1	0.1	0.0	0.0	0.1	0.3	0.3	0.2	0.2	0.3
0.7	0.0	0.2	0.3	0.2	0.2	0.8	1.0	0.2	0.1	0.1	0.1	0.2	0.9
1.8	0.2	0.6	0.6	0.2	0.2	0.0	0.0	0.1	0.5	0.2	0.9	0.5	0.1
0.6	0.7	1.7	1.3	0.9	0.8	3.2	1.5	1.9	7.8	4.9	6.6	9.4	12.2
13.9	19.0	22.9	31.5	38.2	13.5	20.2	6.6	7.4	3.4	8.8	11.2	5.2	28.5
19.1	34.5	108.7	105.3	145.4	49.5	7.5	62.9	108.8	83.6	24.0	53.4	105.4	44.2
42.2	69.9	31.6	45.6	32.4	12.6	4.8	49.6	0.7	27.9	43.9	81.0	24.1	8.7
85.9	46.2	46.6	51.8	8.1	13.3	10.5	57.6	48.3	6.6	26.2	72.1	26.7	52.0
6.9	45.0	71.0	23.1	21.9	28.8	28.5	123.2	49.5	63.6	41.6	104.4	21.7	96.1
11.6	77.3	69.1	19.6	12.8	32.1	21.1	71.0	6.5	7.0	7.5	4.4	13.3	16.1
9.8	0.4	21.3	1.7	0.6	23.4	16.2	57.8	11.4	26.2	27.3	16.6	2.9	9.8
15.3	15.4	11.2	31.1	12.8	2.3	11.2	16.7	8.1	3.5	3.6	33.6	33.9	3.2
16.1	4.3	36.6	0.7	0.6	260.8	136.0							

2.4 Hydrogen at Substitutional Beryllium Atoms

- $H_{AB_\perp}$-Be_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153132.9390213	0.1666455

relaxed coordinates in Å:

H	2.02459690	4.45915540	−1.02026070	O	−1.69217140	6.60590180	−0.65596990
O	−1.65150900	2.79479790	1.98039250	Zn	1.63418370	0.90968730	−2.60169520
O	1.66971810	0.89039840	−0.61406640	Zn	1.60860010	0.88947080	2.66764790
O	−0.03335900	−0.01777910	1.97878510	O	1.62093250	0.94857580	4.65558920
Zn	−0.02296400	3.75772640	−2.59248120	O	1.60308610	2.79639000	−3.20514020
Zn	1.60906030	6.58437940	−2.59247770	O	−0.04030780	5.65216760	−3.23170610
Zn	1.52723250	2.68104260	0.12250800	O	0.01553210	3.77499240	−0.59454990
Zn	−0.06140320	5.66472100	0.03117670	O	1.61360220	6.54288370	−0.59476410
Zn	−0.02045750	3.74219760	2.65736420	O	1.63774280	2.78927430	2.06843800
Zn	1.62394700	6.59002850	2.65749250	O	0.01600810	5.61983740	2.01175020
Zn	1.63868890	2.81847470	5.27696160	O	0.01457600	3.73808930	4.65089720
O	1.64501540	6.56170920	4.65102440	O	1.60539050	2.80177010	7.30021340
O	1.62882160	8.47621050	1.98041280	Zn	4.89733350	0.94046100	−2.53083310
O	3.29010770	−0.03653420	−3.21450150	O	3.26492590	−1.90947580	−0.64652890
Zn	3.31047430	0.00002190	0.01870910	O	4.90825850	1.17405170	−0.50109750
Zn	4.90244800	0.93237920	2.61522300	O	3.26294590	0.01342300	1.99905360
O	4.88376680	0.95954110	4.60721920	Zn	3.27988200	3.73533130	−2.76407720
O	4.91176750	2.79341370	−3.20431060	Zn	4.90430760	6.57334370	−2.60163830
O	3.25475400	5.65703540	−3.20510530	Be	5.26360940	2.59043880	0.18531280
O	2.85203870	3.98212630	−0.75311530	Zn	3.31631750	5.78007000	0.12226570
O	4.93817980	6.55231270	−0.61408030	Zn	3.31381100	3.71593320	2.60143730
O	4.93451780	2.78034450	1.75107460	Zn	4.90872650	6.60566950	2.66781600
O	3.27819300	5.63063590	2.06816180	Zn	4.89073460	2.80537320	5.30409730
O	3.28172930	3.73423000	4.61805450	Zn	3.25339630	5.61497380	5.27725440
O	4.86381550	6.56536590	4.65574960	O	4.90158560	2.79917370	7.31094280
O	3.25123080	5.65240770	7.30055390	O	4.87369510	8.48117230	1.97877280
O	6.54090620	−0.02193310	1.97165030	Zn	6.50928610	3.73212730	−2.53056170
O	6.55184050	5.61245760	−3.21444750	O	6.31244140	3.60638290	−0.50081690
Zn	6.52989630	5.57678400	0.01890530	O	8.16105040	6.57065440	−0.64642950
Zn	6.51888940	3.73183620	2.61538500	O	8.16447430	2.79008270	1.97162560
O	6.49469170	5.61113390	1.99931860	O	6.48583910	3.73430110	4.60732240

calculated wave numbers in cm^{-1} (unscaled):													
90	91	95	96	96	97	103	106	107	108	110	111	114	114
116	119	121	121	122	128	128	131	133	133	137	138	138	139
140	142	144	144	147	150	154	155	158	161	162	178	181	184
185	190	191	196	197	197	198	200	204	207	212	212	216	220
222	226	230	233	236	237	243	244	248	253	264	332	341	346
387	390	400	400	406	421	427	431	435	437	437	440	442	442
443	447	449	449	451	452	452	453	453	455	456	456	457	457
458	461	462	462	463	464	464	467	467	468	469	470	470	472
472	473	473	476	477	478	479	480	480	482	484	484	486	488
489	490	490	492	494	495	496	497	498	500	500	502	504	504
506	506	508	510	516	516	517	517	519	520	523	524	525	526
526	528	528	530	531	532	533	533	534	536	537	537	540	540
542	543	544	546	549	551	551	552	553	561	565	569	618	835
840	885	905	3413										

IR intensities in km/mol:													
0.0	0.1	0.0	0.1	0.0	0.1	0.3	0.1	0.0	0.1	0.0	0.0	0.0	0.1
0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.1	0.1	0.0	0.6	0.0	0.0
0.2	0.0	0.6	0.6	0.5	0.9	0.0	0.1	0.1	0.1	0.6	0.4	0.2	0.4
0.2	2.4	0.1	0.0	0.1	0.0	0.1	0.7	1.1	0.2	0.1	2.1	0.1	0.1
1.1	1.8	0.9	0.2	4.5	1.7	4.4	1.5	13.8	9.2	0.5	22.2	13.2	22.9
5.4	2.4	1.2	53.0	28.9	0.5	39.1	0.2	44.4	0.8	0.4	70.7	70.0	24.0
176.2	41.5	11.1	3.5	2.6	87.7	3.6	31.1	10.8	97.5	12.9	412.5	2.3	4.2
84.4	7.3	14.5	43.8	46.7	5.9	123.7	19.7	30.8	28.9	35.9	48.0	5.7	128.1
0.1	18.3	22.4	6.9	108.0	61.5	41.9	1.4	3.6	9.7	23.9	4.8	6.5	5.2
40.7	74.7	25.0	69.9	5.5	125.9	13.5	7.4	15.9	127.8	141.3	46.4	2.6	20.8
2.5	21.4	96.2	9.6	9.2	8.5	12.4	0.1	4.1	2.2	16.6	34.2	1.6	12.1
24.8	46.9	3.6	2.2	5.1	0.2	4.6	105.9	6.7	10.0	2.0	27.0	2.2	2.1
4.8	0.7	21.3	38.1	7.3	19.5	17.8	20.0	15.8	7.2	30.4	32.2	5.2	38.6
41.6	13.3	5.4	21.4										

- $H_{BC_{\parallel}}$-Be_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153132.9502405	0.1652577

relaxed coordinates in Å:

H	4.50659660	3.03017240	1.24061360	O	−1.67623070	6.59667780	−0.65176990
O	−1.66862580	2.78799010	1.97662890	Zn	1.61145010	0.92570140	−2.57821530
O	1.66087060	0.93040290	−0.59667440	Zn	1.60270700	0.91832690	2.62682780
O	−0.03621860	−0.02054840	1.98004170	O	1.62292250	0.94954410	4.63116790
Zn	−0.02280390	3.76386240	−2.56580320	O	1.61518820	2.81318080	−3.18446100
Zn	1.60382600	6.58119990	−2.56576120	O	−0.04022820	5.65214810	−3.23053580
Zn	1.72979540	2.80829080	0.02745470	O	0.07109920	3.74517320	−0.57450560
Zn	−0.02506740	5.64348170	0.00951120	O	1.66706700	6.50931940	−0.57448580
Zn	−0.04109790	3.74007260	2.62122350	O	1.62713660	2.81558800	2.02452430
Zn	1.61515030	6.60901310	2.62137730	O	0.00873730	5.62388340	2.00082800
Zn	1.58077550	2.79057310	5.32678420	O	0.00854030	3.74017480	4.62958740
O	1.64017530	6.56587920	4.62971580	O	1.59788510	2.79777250	7.33306180
O	1.62613440	8.49440570	1.97662700	Zn	4.86304050	0.88644690	−2.62249670
O	3.24107370	−0.05162230	−3.23431370	O	3.26541000	−1.90850960	−0.64862150
Zn	3.30512130	0.01799800	−0.01812030	O	4.91264830	1.15232880	−0.60164410
Zn	4.88432490	0.87446990	2.65195730	O	3.25917150	0.01294690	1.97108790
O	4.88403900	0.96129050	4.63504260	Zn	3.23199900	3.76305360	−2.61084240
O	4.89315040	2.80393990	−3.15026450	Zn	4.87901150	6.58500020	−2.57819210
O	3.24617440	5.63810190	−3.18446660	Be	4.96082890	2.76481320	−0.68134020
O	3.55652810	3.57586590	−0.53713500	Zn	3.30777280	5.54147150	0.02765830
O	4.89975510	6.53990340	−0.59658060	Zn	3.08678910	3.84667070	2.84581660
O	4.79211980	2.86315550	2.17141490	Zn	4.88085790	6.59634950	2.62712160
O	3.24995120	5.62655920	2.02489630	Zn	4.88486450	2.80864390	5.32275850
O	3.23188950	3.76284060	4.79900920	Zn	3.24856590	5.67896530	5.32702570
O	4.86388450	6.56311380	4.63131630	O	4.90220070	2.79880960	7.32800290
O	3.25095830	5.66099810	7.33336940	O	4.87468010	8.48497290	1.98003070
O	6.52871390	−0.01204050	1.97408820	Zn	6.53866100	3.78869560	−2.62241140
O	6.54030880	5.66239410	−3.23428210	O	6.33324810	3.61288950	−0.60155630
Zn	6.51199170	5.57208670	−0.01790370	O	8.16051130	6.56973900	−0.64853410
Zn	6.56031970	3.77662890	2.65264010	O	8.14982630	2.79565240	1.97411620
O	6.49317250	5.61460340	1.97141700	O	6.48439070	3.73314750	4.63550100

calculated wave numbers in cm^{-1} (unscaled):													
85	91	93	94	96	98	101	106	108	110	110	111	112	113
116	120	120	121	123	125	129	131	132	133	135	135	136	139
141	141	142	142	149	149	151	152	156	158	158	165	176	178
182	185	191	191	196	196	196	199	199	207	208	212	218	219
224	226	228	231	232	242	242	246	250	253	293	316	322	348
365	370	382	388	389	396	417	424	427	431	432	436	436	439
439	442	442	443	444	449	450	451	452	452	454	455	457	458
458	460	462	462	463	464	465	465	468	468	470	471	471	472
473	474	475	476	477	478	478	480	482	482	483	483	485	486
486	488	489	489	490	491	492	493	497	499	500	502	502	503
505	505	506	508	510	511	514	515	515	516	518	519	520	523
524	525	527	527	528	528	529	530	532	533	533	539	541	543
543	545	545	547	549	550	553	553	554	555	578	580	610	645
798	844	897	3472										

IR intensities in km/mol:													
0.3	0.1	0.0	0.1	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.3	0.0	0.2
0.0	0.0	0.0	0.0	0.1	0.2	0.2	0.1	0.0	0.0	0.1	0.1	0.3	0.0
0.1	0.2	0.7	0.1	0.0	0.4	0.5	0.1	0.1	0.2	0.0	0.0	0.6	1.8
1.1	0.4	0.2	0.3	0.2	0.9	0.2	0.3	0.3	1.0	2.1	0.1	1.3	0.1
0.0	3.2	4.3	5.0	1.2	3.2	4.4	6.7	2.2	10.7	2.1	18.8	8.3	18.3
23.0	26.5	34.9	2.6	29.0	0.3	8.6	0.3	103.6	1.5	30.4	100.2	113.3	25.0
106.8	0.4	92.4	129.4	1.1	17.2	16.8	0.3	29.0	1.2	27.5	8.9	1.1	34.0
0.2	10.6	182.1	95.6	60.9	16.3	128.6	50.1	37.0	11.2	36.2	0.3	3.5	55.6
51.1	69.7	23.8	0.3	2.9	13.9	0.6	164.0	38.1	69.3	13.4	31.8	50.4	7.9
0.5	40.1	64.2	23.6	88.0	48.1	42.3	48.7	0.8	13.4	37.5	4.7	140.7	13.7
0.7	17.6	76.6	0.1	33.6	0.3	34.8	39.9	74.1	16.4	9.4	49.0	31.7	18.1
8.6	24.8	5.5	34.3	102.6	13.6	21.1	1.5	13.6	5.7	0.2	8.6	30.4	2.0
19.0	7.7	7.3	14.5	10.4	9.8	8.4	8.8	0.0	17.4	34.3	38.4	0.5	0.2
39.3	40.8	6.3	57.8										

- $H_{BC_\perp}$-Be_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153132.9466818	0.1652265

relaxed coordinates in Å:

H	3.97780400	3.32440750	−0.74203660	O	−1.69361680	6.60678000	−0.65687460
O	−1.65108270	2.79448530	1.98187200	Zn	1.63136050	0.90242640	−2.59129520
O	1.66745940	0.92004550	−0.60625900	Zn	1.60591260	0.91413820	2.64247570
O	−0.03323010	−0.01838270	1.97849970	O	1.62175690	0.94996990	4.63884770
Zn	−0.03674260	3.77159630	−2.57778920	O	1.56321910	2.78363950	−3.21215170
Zn	1.59025080	6.58946910	−2.57763060	O	−0.04393900	5.65439800	−3.23709110
Zn	1.56378140	2.77256860	0.03781250	O	0.00225340	3.78194890	−0.59469040
Zn	−0.05704800	5.66234390	0.02367620	O	1.60174090	6.55020230	−0.59468230
Zn	−0.00824970	3.73862910	2.63910900	O	1.65005700	2.80371890	2.01221880
Zn	1.63329540	6.58117640	2.63894160	O	0.01420140	5.62085990	2.00724530
Zn	1.63553990	2.81698750	5.27176520	O	0.01522320	3.73783850	4.63897250
O	1.64555600	6.56128880	4.63889420	O	1.60514680	2.80167140	7.29628360
O	1.62930110	8.47599140	1.98184200	Zn	4.89692550	0.96002460	−2.53558290
O	3.29401480	−0.03265570	−3.21081340	O	3.26460900	−1.90307100	−0.64509580
Zn	3.29707000	0.00898220	0.02249440	O	4.91535240	1.18927840	−0.48334360
Zn	4.90238700	0.90571230	2.64371810	O	3.26341690	0.01348440	2.00195050
O	4.88418110	0.95893210	4.62634020	Zn	3.18209520	3.79173410	−2.82905750
O	4.85897990	2.82384490	−3.19018710	Zn	4.90913310	6.57934850	−2.59144590
O	3.24567150	5.69764150	−3.21211740	Be	5.38588380	2.52101830	0.29116240
O	3.13182010	3.81940280	−0.74285740	Zn	3.25670800	5.70121680	0.03711340
O	4.91203780	6.53956670	−0.60647130	Zn	3.31688640	3.71405580	2.59459430
O	4.98002470	2.75449360	1.80826570	Zn	4.88587610	6.59572740	2.64258430
O	3.27191890	5.61243310	2.01166110	Zn	4.88427440	2.80904650	5.30815900
O	3.27988490	3.73530060	4.61052990	Zn	3.25308600	5.61848170	5.27197760
O	4.86300940	6.56396160	4.63892320	O	4.90040080	2.79985080	7.31408610
O	3.25119030	5.65266480	7.29656160	O	4.87426730	8.48138220	1.97846860
O	6.54377100	−0.02527620	1.97152980	Zn	6.49207350	3.72278740	−2.53529150
O	6.55043750	5.60714610	−3.21085860	O	6.30442300	3.59320820	−0.48325750
Zn	6.51587240	5.58404280	0.02266700	O	8.15560200	6.56790220	−0.64507530
Zn	6.54227070	3.74561770	2.64422950	O	8.16881740	2.78929330	1.97163300
O	6.49485090	5.61094440	2.00226510	O	6.48656320	3.73426390	4.62666870

calculated wave numbers in cm^{-1} (unscaled):													
89	93	93	96	97	102	105	107	110	111	112	112	114	116
118	121	122	123	128	130	131	132	132	137	137	138	139	140
141	143	144	147	149	153	155	158	159	162	165	175	179	185
186	190	192	194	196	197	198	204	205	211	212	216	216	223
227	229	230	235	240	241	245	246	251	255	300	319	352	356
379	385	386	394	418	426	432	433	435	436	437	437	439	441
445	447	447	448	450	450	451	452	453	454	455	456	457	457
458	460	462	462	463	463	464	466	467	468	470	471	472	472
473	474	475	476	476	478	478	480	482	482	484	485	485	486
487	489	490	491	492	492	496	498	499	501	501	502	502	505
506	508	510	511	514	517	517	518	519	521	522	523	524	524
526	529	529	531	533	533	534	535	536	537	538	538	539	540
541	542	543	545	545	548	548	551	554	560	564	569	612	821
833	880	3613											

IR intensities in km/mol:													
0.2	0.3	0.1	0.1	0.0	0.0	0.1	0.0	0.2	0.0	0.0	0.0	0.1	0.0
0.1	0.0	0.0	0.0	0.0	0.2	0.0	0.1	0.1	0.1	0.2	0.4	0.0	0.0
0.4	0.0	0.9	0.3	0.9	0.1	0.1	0.1	0.0	0.8	0.3	1.0	1.1	0.0
0.8	0.7	0.2	0.5	0.0	0.0	0.1	0.2	1.1	0.2	0.8	0.3	0.2	1.8
1.8	1.0	0.2	4.8	4.4	1.6	2.1	0.1	9.6	9.7	15.4	17.2	18.0	18.7
4.4	46.5	7.3	4.5	0.7	72.1	1.2	0.7	32.8	17.7	48.9	76.4	54.0	2.6
116.7	44.7	20.1	6.1	40.7	12.1	0.0	35.3	90.9	1.5	7.0	255.8	121.3	60.1
1.1	120.7	49.3	25.3	13.8	46.5	89.0	14.3	13.3	18.4	17.2	35.5	37.4	3.0
165.4	114.1	3.7	6.1	82.3	10.2	21.4	2.2	13.4	9.8	18.4	31.8	5.7	23.3
54.0	0.5	50.0	122.3	53.5	69.0	17.6	53.9	28.9	158.9	40.2	51.2	6.6	38.4
5.4	113.6	8.0	0.2	2.4	19.1	6.0	10.8	27.4	4.8	14.0	35.6	6.1	14.0
16.9	0.2	3.7	44.7	0.5	0.9	1.7	0.4	5.9	22.3	27.3	9.8	4.1	6.3
28.2	20.6	8.0	18.1	71.6	19.7	55.5	11.5	1.4	10.7	36.2	33.8	3.5	7.1
30.8	28.3	32.3											

2.5 Hydrogen at Substitutional Magnesium Atoms

- $H_{AB_{\parallel}}$-Mg_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153318.1683129	0.1644833

relaxed coordinates in Å:

H	3.06498360	3.86589230	0.60040320	O	−1.69771060	6.60906940	−0.65923080
O	−1.64958970	2.79499660	1.97918020	Zn	1.63240420	0.89557310	−2.60620880
O	1.66387130	0.88005360	−0.62271810	Zn	1.61096230	0.92551580	2.64253830
O	−0.02937770	−0.01194110	1.97880850	O	1.61946090	0.95539250	4.63843410
Zn	−0.03358140	3.77544370	−2.60162210	O	1.60576130	2.80347530	−3.17266480
Zn	1.58779070	6.58456020	−2.60261590	O	−0.04845260	5.65644180	−3.24558140
Zn	1.42595730	2.68414950	0.02108680	O	−0.02023120	3.79764730	−0.61876350
Zn	−0.06815660	5.66783300	0.02920700	O	1.57455090	6.56261300	−0.61986610
Zn	−0.01379260	3.74145740	2.64480440	O	1.65221700	2.82844210	1.99777520
Zn	1.62788170	6.58391860	2.64430410	O	0.01268340	5.62145030	2.00670470
Zn	1.60348890	2.80191150	5.31624900	O	0.01243990	3.73864500	4.64039930
O	1.64350260	6.56327150	4.63989820	O	1.59981470	2.79994050	7.32447450
O	1.62969000	8.47409710	1.97912080	Zn	4.87548470	0.89697050	−2.57880790
O	3.25754920	−0.05514120	−3.24449220	O	3.25094830	−1.96482440	−0.66042190
Zn	3.27381680	−0.08341910	0.02295400	O	4.85451710	0.92546830	−0.59754970
Zn	4.90021100	0.92465540	2.65281960	O	3.25547700	0.01395310	2.00529270
O	4.88079910	0.95445280	4.64756070	Zn	3.23287440	3.76265100	−2.73199300
O	4.87837620	2.81252780	−3.14919690	Zn	4.91596630	6.58185980	−2.60702860
O	3.24991810	5.65143570	−3.17249540	Mg	4.97277680	2.75762240	0.03723320
O	3.24739960	3.75410170	−0.37502650	Zn	3.26310290	5.87042020	0.01853120
O	4.94583920	6.56295560	−0.62360290	Zn	3.28120980	3.73387110	2.77631820
O	4.87897600	2.81231600	2.01249140	Zn	4.87868140	6.58493600	2.64207420
O	3.25145080	5.59767700	1.99535080	Zn	4.89764050	2.80145820	5.31983820
O	3.25116520	3.75211340	4.74399960	Zn	3.25017820	5.65404670	5.31646710
O	4.85715180	6.56322060	4.63789210	O	4.89999740	2.80011790	7.32750400
O	3.25005920	5.65830300	7.32470650	O	4.87057460	8.47446980	1.97873480
O	6.53468260	−0.01626810	1.98001160	Zn	6.53582720	3.77251280	−2.57865710
O	6.55189310	5.64970430	−3.24456090	O	6.50041780	3.77630640	−0.59735530
Zn	6.58437990	5.64957580	0.02297750	O	8.20208950	6.61048500	−0.66028330
Zn	6.52437370	3.73746070	2.65287700	O	8.15645510	2.79261450	1.97996400
O	6.49067330	5.61708010	2.00523670	O	6.48878150	3.73948330	4.64753990

calculated wave numbers in cm^{-1} (unscaled):													
61	82	88	90	95	95	97	98	104	107	109	111	111	112
115	116	119	120	121	122	126	127	131	132	133	136	136	139
139	140	141	142	145	146	149	151	152	158	159	162	183	185
186	186	192	194	196	197	198	203	206	209	210	218	218	222
224	225	228	231	232	240	242	246	248	251	257	273	276	297
319	395	411	416	425	426	432	435	437	439	440	441	441	446
446	447	450	450	451	453	454	455	457	457	458	458	460	461
462	462	463	463	464	465	467	468	469	470	472	474	475	475
477	477	478	478	479	480	482	482	484	485	485	486	487	490
491	494	494	494	495	497	501	501	502	503	504	505	505	507
510	513	514	516	516	518	519	520	521	522	523	525	526	529
529	531	532	532	533	534	535	536	536	541	541	543	544	546
548	549	550	550	550	551	554	557	560	561	569	575	576	582
606	744	823	3271										

IR intensities in km/mol:													
1.8	2.5	0.3	0.1	0.0	0.1	0.0	0.4	0.0	0.3	0.1	0.1	0.0	0.0
0.1	0.1	0.1	0.4	0.2	0.2	0.1	0.3	0.0	0.0	0.1	0.0	0.3	0.1
0.5	0.2	0.2	0.1	0.1	1.4	0.1	0.6	0.1	0.0	0.1	0.0	0.8	0.3
1.0	1.1	0.1	0.2	0.4	0.1	0.0	0.1	1.9	0.4	1.5	0.4	0.6	1.9
0.2	0.2	0.1	0.1	0.6	0.0	4.6	10.2	9.1	12.3	3.5	1.4	15.4	2.8
5.4	18.8	0.2	47.0	200.5	44.5	5.0	41.9	0.4	4.1	0.3	0.8	10.1	10.6
9.7	0.5	26.1	1.1	6.9	68.1	8.0	248.7	33.6	2.6	78.3	74.3	3.4	227.3
2.5	39.4	70.3	16.1	49.7	48.1	85.7	64.7	48.0	88.2	0.5	46.9	120.0	111.3
13.3	6.8	27.8	30.6	15.0	41.3	4.3	111.3	31.2	214.0	18.2	9.4	55.8	7.4
6.7	78.0	5.2	6.5	23.0	14.9	66.6	5.4	3.3	34.0	48.1	19.2	22.7	114.8
25.2	19.1	5.7	17.3	1.8	26.1	87.4	7.5	72.0	62.1	7.6	8.2	0.0	15.4
0.2	2.6	70.7	10.5	2.5	11.7	4.8	0.0	0.8	55.1	90.4	0.4	41.0	19.9
5.9	6.5	0.1	0.3	9.7	2.1	36.8	10.9	14.8	12.9	20.3	42.2	42.2	19.0
27.9	1.2	3.7	58.3										

- $H_{AB_{\perp}}$-Mg_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153318.1737653	0.1641909

relaxed coordinates in Å:

H	2.28978960	4.30921230	−0.97580290	O	−1.68464840	6.60158480	−0.65481900
O	−1.65484240	2.79454440	1.97693700	Zn	1.62836980	0.90417890	−2.58914540
O	1.66837400	0.89072260	−0.60306440	Zn	1.60672250	0.88777660	2.67984920
O	−0.03403660	−0.01596760	1.97921490	O	1.61828180	0.95135570	4.66502300
Zn	−0.02490090	3.76341220	−2.58880090	O	1.60677690	2.79933220	−3.19187480
Zn	1.60317050	6.58321730	−2.58890790	O	−0.04125300	5.65275160	−3.23373470
Zn	1.47406640	2.65342740	0.17223760	O	0.04470700	3.77123320	−0.59327350
Zn	−0.05331730	5.65994670	0.03370450	O	1.63184530	6.51907540	−0.59330430
Zn	−0.04035560	3.74987120	2.67275670	O	1.61890760	2.79959450	2.10207460
Zn	1.60709290	6.60345100	2.67311200	O	0.01386140	5.62104330	2.01304400
Zn	1.61563460	2.80856380	5.31294280	O	0.00986400	3.73964650	4.66046890
O	1.64126170	6.56504220	4.66071910	O	1.60106260	2.80047140	7.32434500
O	1.62736410	8.47919610	1.97692630	Zn	4.87815990	0.88242260	−2.56512100
O	3.25217150	−0.05205510	−3.23906150	O	3.25214290	−1.96388170	−0.66011370
Zn	3.27956310	−0.08516530	0.02470490	O	4.84181880	0.96339580	−0.58485290
Zn	4.89769450	0.94701850	2.62869500	O	3.25262190	0.01318600	2.00699510
O	4.88110610	0.95476230	4.62969560	Zn	3.28684840	3.73089740	−2.87205440
O	4.93440720	2.78001480	−3.17774330	Zn	4.90586190	6.58102640	−2.58915920
O	3.25389860	5.65189290	−3.19165520	Mg	4.83287910	2.83895040	−0.01151980
O	3.09697510	3.84025940	−0.64400360	Zn	3.31422370	5.84055240	0.17311770
O	4.93723460	6.55335130	−0.60313840	Zn	3.25999450	3.74679990	2.73066970
O	4.84661820	2.83105950	1.96381980	Zn	4.90961310	6.60814950	2.68020530
O	3.25981880	5.64181770	2.10256700	Zn	4.89587490	2.80245850	5.30881560
O	3.25556700	3.74943060	4.72316600	Zn	3.25044930	5.64000010	5.31328600
O	4.86011890	6.56628000	4.66521860	O	4.90097730	2.79954010	7.32010230
O	3.25021200	5.65689530	7.32472880	O	4.87181690	8.48081180	1.97920910
O	6.53206650	−0.01513020	1.97931560	Zn	6.54967040	3.77767170	−2.56533550
O	6.54617890	5.65322140	−3.23899980	O	6.46163980	3.76883590	−0.58508180
Zn	6.58825700	5.64600280	0.02454450	O	8.20178230	6.60900450	−0.65995660
Zn	6.50385460	3.72861390	2.62877530	O	8.15416370	2.79432810	1.97925900
O	6.48978980	5.62007170	2.00693280	O	6.48866120	3.73905960	4.62966700

calculated wave numbers in cm^{-1} (unscaled):													
55	76	90	93	96	96	99	102	109	109	110	111	113	113
115	116	119	120	120	124	125	130	131	132	135	136	137	138
140	141	142	144	147	150	151	153	158	158	162	162	179	179
186	187	192	194	196	198	198	201	201	209	211	215	218	222
226	228	228	231	233	235	242	245	246	247	249	264	285	298
298	342	404	411	423	424	427	428	431	435	438	439	440	443
446	448	449	449	451	452	453	455	455	456	457	459	460	462
462	463	463	464	465	466	466	467	467	470	472	474	475	476
476	477	478	479	480	482	482	483	484	485	485	486	487	488
489	492	494	494	495	496	499	499	501	502	502	503	507	508
509	512	513	515	517	518	519	520	521	524	524	526	528	528
529	531	532	533	534	535	536	537	538	538	539	539	544	546
548	548	549	550	551	552	553	555	557	561	564	572	575	576
582	722	756	3399										

IR intensities in km/mol:													
2.1	4.8	0.2	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.0	0.1	0.0
0.0	0.0	0.1	0.0	0.0	0.1	0.0	0.0	0.1	0.0	0.1	0.0	0.1	0.1
0.0	0.1	1.3	0.0	1.1	0.8	0.1	0.0	0.1	0.3	0.0	0.4	0.1	0.7
0.0	0.6	0.0	1.3	0.8	0.0	0.2	0.6	1.2	0.7	2.2	0.1	1.9	0.1
1.1	2.6	1.6	3.2	2.2	4.8	11.7	9.4	8.7	10.6	7.7	11.3	7.8	2.5
0.1	4.8	5.8	11.8	99.0	9.8	8.9	19.2	5.7	68.7	28.5	75.2	11.6	32.2
96.8	52.0	11.8	0.1	37.2	2.3	0.2	89.9	24.7	41.0	163.6	248.2	19.8	20.6
3.2	173.3	5.1	85.0	20.4	99.9	55.3	34.5	22.4	2.9	57.3	31.1	75.1	133.8
56.4	54.5	3.3	5.7	59.0	7.9	38.1	6.8	21.6	35.3	5.8	25.2	154.9	68.1
10.6	32.5	8.8	42.5	12.4	7.2	12.4	15.0	81.4	16.2	143.0	0.1	26.7	97.1
103.2	15.5	38.0	38.0	2.9	24.5	21.9	43.8	16.8	34.1	0.3	0.2	13.1	12.3
11.8	8.6	0.0	2.7	44.9	7.8	0.2	0.2	7.7	84.4	4.6	8.9	2.6	3.5
9.1	18.8	0.1	0.8	17.5	17.0	3.4	49.8	21.0	17.9	16.0	36.4	44.3	36.5
22.9	2.7	2.5	34.0										

- $H_{BC_{\parallel}}$-Mg_{Zn}

Energy (a.u.)	ZPVE (a.u.)
-153318.1643855	0.1651037

relaxed coordinates in Å:

H	4.34380070	3.11961700	1.24749640	O	−1.69139140	6.60544310	−0.65570630
O	−1.67118360	2.78690200	1.97844600	Zn	1.59401010	0.92965400	−2.56207160
O	1.64959750	0.94068180	−0.58379230	Zn	1.58784320	0.91776690	2.64443560
O	−0.04072250	−0.02207550	1.98033830	O	1.62128940	0.95128390	4.64530630
Zn	−0.03957590	3.77176900	−2.56589580	O	1.58160730	2.80373080	−3.20115320
Zn	1.58852200	6.59181030	−2.56581760	O	−0.04340270	5.65396760	−3.23493290
Zn	1.63080670	2.81994740	0.05910040	O	0.01434030	3.77232400	−0.58181510
Zn	−0.05046640	5.65813750	0.01739400	O	1.61514580	6.54485740	−0.58182050
Zn	−0.05944020	3.74555900	2.64030730	O	1.60633200	2.81515030	2.05712430
Zn	1.60133580	6.62214780	2.64037810	O	0.00885130	5.62384710	2.00738790
Zn	1.58075310	2.78981440	5.33683340	O	0.00869020	3.74082640	4.64231120
O	1.63968400	6.56541590	4.64238490	O	1.59818800	2.79807660	7.33977770
O	1.62580560	8.49718210	1.97843070	Zn	4.83265910	0.79752320	−2.65864940
O	3.19171140	−0.06758160	−3.25714760	O	3.25071830	−1.96288880	−0.66128650
Zn	3.24057300	−0.06861310	0.00573060	O	4.85329080	0.86410510	−0.64968780
Zn	4.87164510	0.87897490	2.63320410	O	3.23480700	0.01159070	1.99153060
O	4.88273870	0.96263890	4.61968410	Zn	3.13630580	3.81839380	−2.61978310
O	4.88024940	2.81158710	−3.00746470	Zn	4.86673920	6.59811270	−2.56225290
O	3.23738340	5.67203940	−3.20127970	Mg	4.94361770	2.77519730	−0.81294900
O	3.28921720	3.73016440	−0.54883600	Zn	3.24825710	5.62135370	0.05919210
O	4.88493490	6.54470250	−0.58409710	Zn	3.05496630	3.86531340	2.86930560
O	4.77197320	2.87390110	2.10384430	Zn	4.87399010	6.60957190	2.64476920
O	3.24008830	5.64495920	2.05729120	Zn	4.89166050	2.80486760	5.31846870
O	3.23304730	3.76221380	4.81188640	Zn	3.24917590	5.67941590	5.33713250
O	4.86154930	6.56367000	4.64550330	O	4.90317360	2.79827270	7.32421910
O	3.25085360	5.66060960	7.34011870	O	4.87376880	8.48967050	1.98031560
O	6.52552660	−0.00606630	1.98012340	Zn	6.60072720	3.85975510	−2.65842590
O	6.52935920	5.71323910	−3.25717660	O	6.55333350	3.80890720	−0.64921690
Zn	6.55441330	5.67187270	0.00588970	O	8.20023410	6.60977750	−0.66114660
Zn	6.54941600	3.78520650	2.63296980	O	8.14288680	2.79544490	1.98014800
O	6.48212170	5.63644050	1.99170300	O	6.48256330	3.73362750	4.61951950

calculated wave numbers in cm^{-1} (unscaled):													
87	91	91	95	95	98	100	104	106	108	110	110	112	112
115	118	119	120	121	123	123	130	130	131	133	134	134	136
139	141	141	142	147	149	150	156	157	158	160	165	170	182
184	186	191	192	194	196	196	199	202	210	211	214	217	222
227	229	232	232	236	243	245	247	251	254	257	297	306	308
344	347	349	357	406	416	425	432	437	438	439	443	445	446
447	449	449	450	451	453	454	455	457	457	459	459	460	461
461	462	464	466	467	467	468	468	469	469	470	472	473	473
475	476	478	478	480	481	481	482	483	484	485	487	490	490
491	492	492	493	497	498	499	500	502	504	505	506	507	511
511	512	514	515	515	516	518	519	519	522	522	524	526	526
527	528	529	532	533	533	533	535	536	537	538	543	543	545
547	548	549	550	553	555	555	557	560	560	578	582	591	616
643	663	975	3438										

IR intensities in km/mol:													
0.4	0.3	0.1	0.4	0.1	0.0	0.0	0.1	0.3	0.1	0.0	0.1	0.1	0.0
0.1	0.0	0.0	0.5	0.0	0.0	0.1	0.1	0.1	0.2	0.0	0.1	0.0	0.0
0.5	0.1	0.3	0.1	0.3	0.2	0.1	0.3	0.1	0.0	0.3	1.3	2.3	0.1
0.0	1.3	0.3	0.3	0.6	0.0	0.2	0.2	0.0	0.1	1.3	0.9	0.7	0.2
1.9	3.6	0.5	2.0	1.4	0.4	2.6	8.0	6.8	12.9	2.3	10.6	2.6	1.2
58.6	17.7	15.8	4.9	2.2	21.0	10.6	47.8	4.6	1.1	15.5	2.3	46.5	284.5
2.0	35.1	32.5	21.9	102.3	10.9	18.8	48.7	23.3	50.0	29.9	166.1	17.9	3.3
38.3	13.4	14.3	4.5	133.9	8.4	18.4	20.1	73.3	23.4	50.1	1.6	45.9	86.3
43.0	28.5	73.3	60.3	0.9	7.0	121.6	119.3	158.4	17.0	63.1	0.1	4.3	0.7
0.4	1.7	26.7	47.4	8.6	55.7	105.7	0.9	39.7	16.0	81.8	39.7	29.8	45.0
54.0	8.8	1.3	6.0	9.9	27.9	0.1	46.8	27.5	39.4	14.4	82.7	3.6	7.4
3.4	7.3	37.1	4.9	5.9	24.1	14.3	46.8	9.1	37.3	130.8	15.9	33.3	9.7
1.7	8.0	25.6	20.4	17.1	0.1	24.6	14.3	1.9	0.5	35.5	38.9	2.4	0.3
16.0	23.1	1.6	79.2										