

Supporting Information for “Theoretical studies of function switch and mechanism of AceK as a highly active ATPase”

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Supplementary computational analyses

Investigations of water wire effect on ATPase reaction

Extensive studies have found that it would be more effective to utilize more than one water molecule to relay and complete proton transfer in hydrolysis reaction.¹⁻⁶ Because in AceK the room between γ -phosphoryl and the proton acceptor Asp457 is able to accommodate two lytic water molecules, we also studied the two-water hydrolysis mechanism of AceK. Similar to that in the single-water mechanism, we found that the dissociative pathway is the favorable one in the two-water mechanism. The calculated energy barriers for associative and dissociative mechanisms are 31.21 kcal·mol⁻¹ and 21.33 kcal·mol⁻¹, respectively. The geometries of reactants, transition states and products are depicted in Figure S2 and key structural parameters are listed in Table S2.

In the two-lytic-water pathway, the second water molecule acts as a bridge between the lytic water and Asp457. When the OH_{wat1} of the lytic water attacks the γ -phosphates of ATP, a proton is transferred to the bridge water, which gives out another proton to Asp457 at the same time (Scheme S1). Comparing to that of Model_{1-wat}, the calculated 21.33 kcal·mol⁻¹ energy barrier indicates that the two-lytic-water pathway for ATPase reaction is energetically unfavorable. For the dissociative structures of the two-lytic-water pathway, the strong hydrogen bonding interaction between the lytic water and O _{γ 2} of ATP (O_{wat1}-O _{γ 2}ATP=2.82 Å) in reactant hinders the movement and nucleophilic attacking of the lytic water, which may contribute to a

higher energy barrier. Furthermore, although there is room to accommodate two water between ATP and Asp457, one more water causes extra steric conflicts in the active site, which would also be a reason of slowing ATP hydrolysis. In conclusion, the dissociative mechanism with one lytic water is the most reasonable and energetically favorable pathway for ATPase reaction.

Investigations of the number of Mg^{2+} in active center on ATPase activity of AceK

It is well known that one important role played by AceK in the cell is its kinase function. Typical kinases such as ePKs usually contain two Mg^{2+} ions (or other metal ions) in their active sites. AceK, however, contains only one Mg^{2+} ion in its active site.

Similar to our previous work on kinase and phosphatase of AceK^{7, 8}, we further investigated ATP hydrolysis using a double- Mg^{2+} model of AceK. In this case, the second Mg^{2+} ion was manually added in the active site with the similar position observed in ePKs. The added Mg^{2+} ion is coordinated with γ -phosphates of ATP and the carboxylate group of Asp457 to balance the local negative charges. In addition, three water molecules are included to complete the coordination of the second Mg^{2+} ion. The final model has a net charge of +1. Similarly, the ATP hydrolysis reaction was analyzed for both associative and dissociative pathways. The geometries of reactants, transition states and products are depicted in Figure S3 and key structural parameters are listed in Table S3.

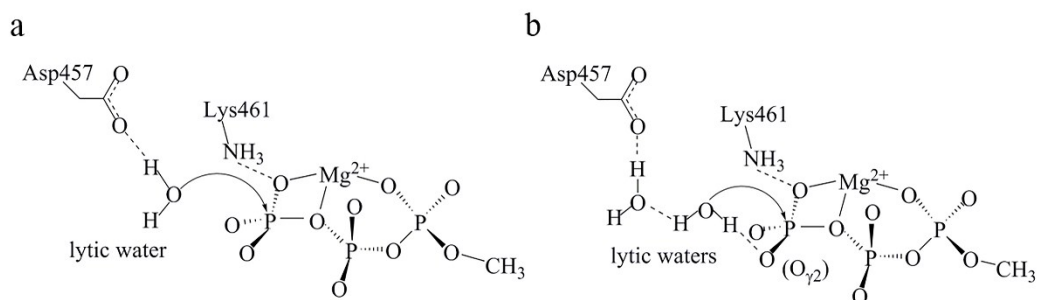
Our results show that the added Mg^{2+} severely hinders ATP hydrolysis with higher energy barriers of $45.91 \text{ kcal}\cdot\text{mol}^{-1}$ for associative mechanism and $29.16 \text{ kcal}\cdot\text{mol}^{-1}$

for the dissociative one. Note that the unique single Mg^{2+} ion in ATPase stabilizes the reactant, transition state and product by its octahedral coordination with α -, β - and γ -phosphoryl groups of ATP, Asn462, Asp475 and one water molecule, same as reported in our kinase study. In the double- Mg^{2+} model, the active site is unable to fully accommodate the octahedral coordination for the second Mg^{2+} ion throughout the reaction. Furthermore, the added Mg^{2+} also makes the space more crowded for the ATP hydrolysis and makes this reaction more difficult to happen.

Further discussion of ATPase and kinase activities of AceK

AceK integrates kinase, phosphatase and ATPase activities at the same active site. Because AceK possesses much higher ATPase activity than the other two activities, it seems reasonable that ATP hydrolysis is the main source for ADP which is essential for its phosphatase activity. In order to gain deeper understanding, the Mulliken charges of critical atoms were analyzed for both ATPase model and kinase model (Table S5). Clearly, P_γ of reactant is more positive in ATPase model than that in kinase model, while O_{wat} of reactant in ATPase model is more negative than O_{ser113} in the kinase model. The stronger electrophilicity of the γ -phosphates in ATP and nucleophilicity of the lytic water may enable AceK to have much higher ATPase activity than its kinase activity.

Scheme S1, Figure S1-S4, Table S1-S5:



Scheme S1. Schematic diagram of proton transfers. a. A direct proton transfer path with one lytic water. b. Water-assisted proton transfer path.

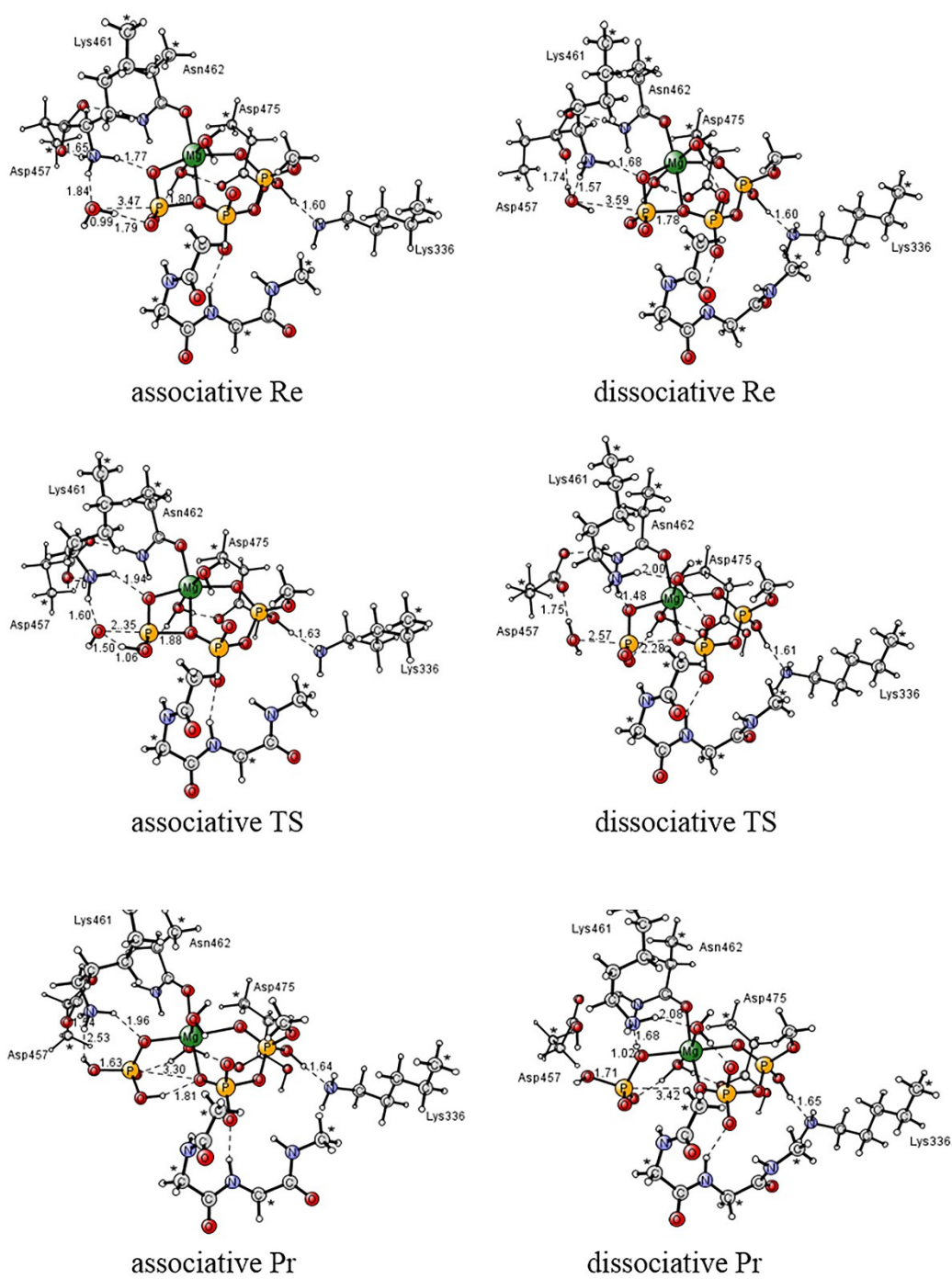


Figure S1. The optimized structures of Re, TS and Pr for the Model_{2-wat} of AceK. Main-chain carbons are marked with asterisks.

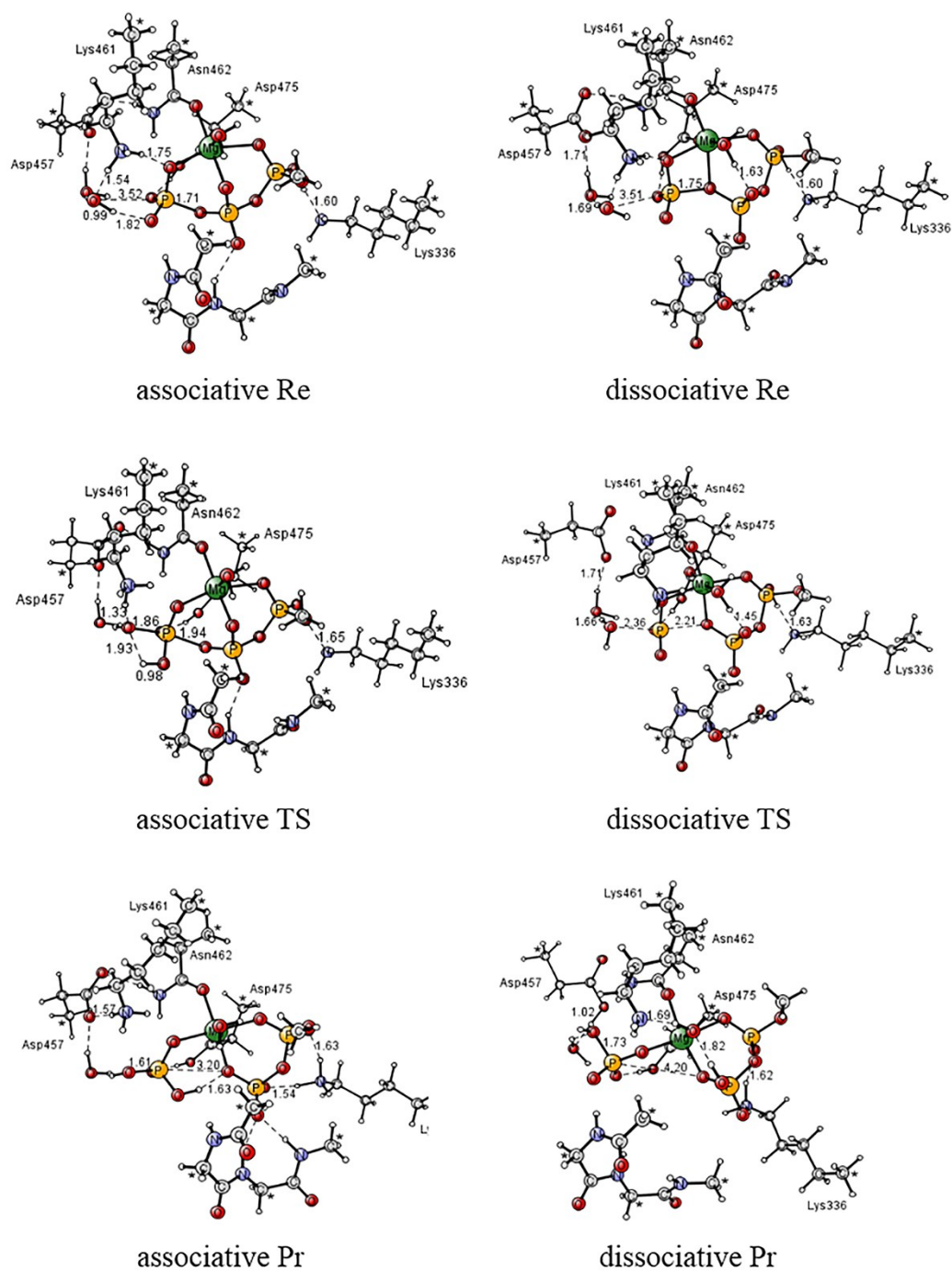
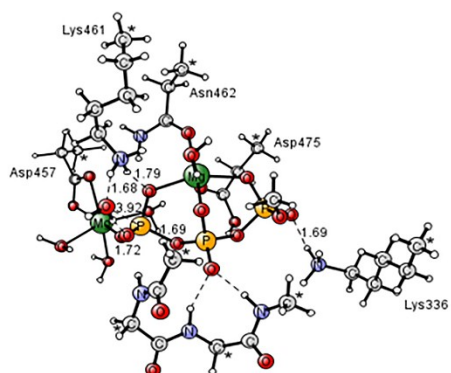
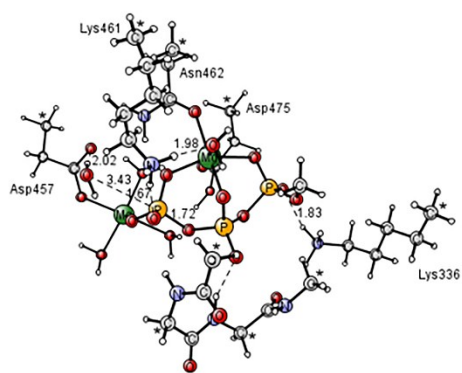


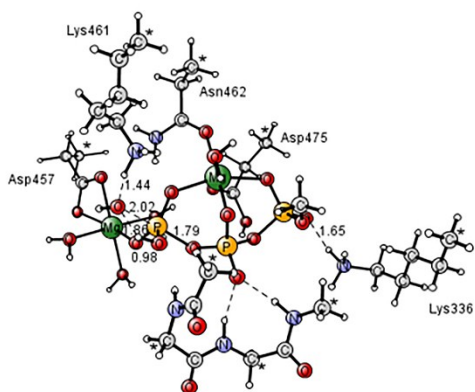
Figure S2. The optimized structures of Re, TS and Pr for the Model_{1-wat} of AceK with one more lytic water. Main-chain carbons are marked with asterisks.



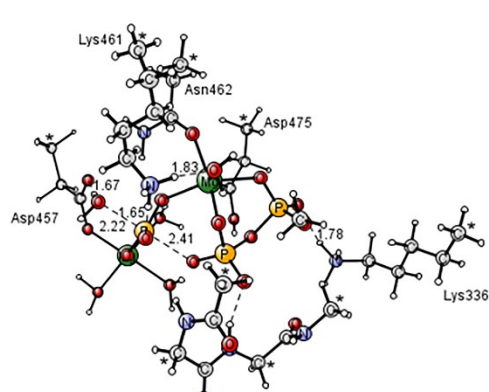
associative Re



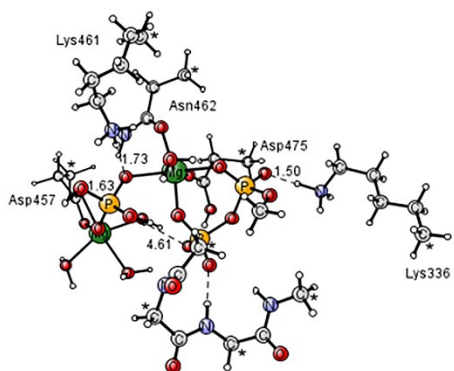
dissociative Re



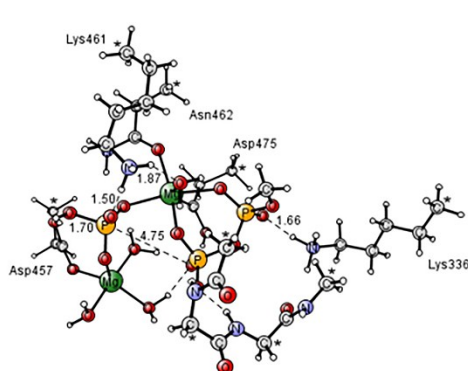
associative TS



dissociative TS



associative Pr



dissociative Pr

Figure S3. The optimized structures of Re, TS and Pr for the double-Mg²⁺ model of AceK. Main-chain carbons are identified with asterisks.

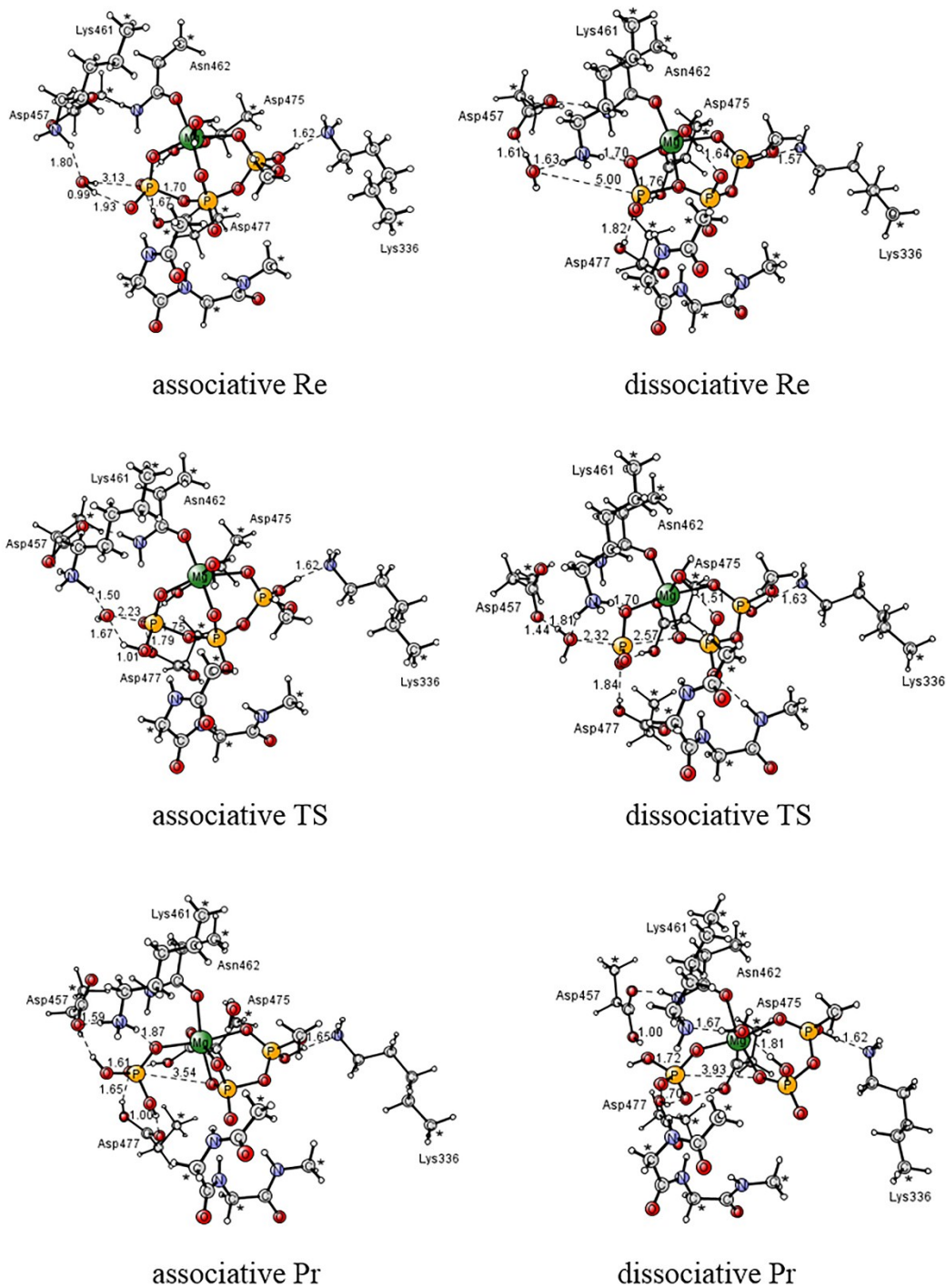


Figure S4. The optimized structures of Re, TS and Pr for the model extracted from AceK-ICDH complex. Main-chain carbons are identified with asterisks.

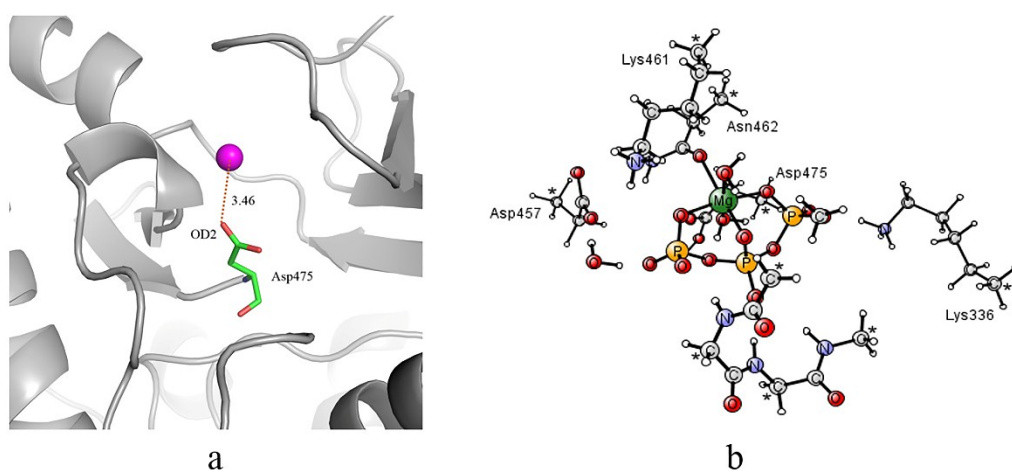


Figure S5. A close-up view of Mg²⁺ with Asp475 (a) and geometry structure of Model_{2-wat} (b) for AceK. Main-chain carbons are identified with asterisks.

Table S1. Important bond lengths (Å) of Re, TS and Pr for Model_{2-wat} of AceK.

	associative			dissociative		
	Re	TS	Pr	Re	TS	Pr
O _{βγ} ATP-P _γ ATP	1.80	1.88	3.30	1.78	2.28	3.42
O _{wat} -P _γ ATP	3.47	2.35	1.63	3.59	2.57	1.71
O _{Asp457} -H _{wat}				1.74	1.75	1.00
H _{wat} -O _{γ2} ATP	1.79	1.06	0.99			

Table S2. Important bond lengths (Å) of Re, TS and Pr for Model_{1-wat} of AceK with one more lytic water.

	associative			dissociative		
	Re	TS	Pr	Re	TS	Pr
O _{βγ} ATP-P _γ ATP	1.71	1.94	3.20	1.75	2.21	4.20
O _{wat1} -P _γ ATP	3.52	1.86	1.61	3.51	2.36	1.73
H _{wat1} -O _{wat2}				1.69	1.66	0.98
O _{Asp457} -H _{wat2}				1.71	1.71	1.02
H _{wat1} -O _{γ2} ATP	1.82	0.98	1.01			

Table S3. Important bond lengths (\AA) of Re, TS and Pr for the double- Mg^{2+} model of AceK.

	associative			dissociative		
	Re	TS	Pr	Re	TS	Pr
$\text{O}_{\beta\gamma}\text{ATP}-\text{P}_{\gamma}\text{ATP}$	1.69	1.79	4.61	1.72	2.41	4.75
$\text{O}_{\text{wat}}-\text{P}_{\gamma}\text{ATP}$	3.92	2.02	1.63	3.43	2.22	1.70
$\text{O}_{\text{Asp457}}-\text{H}_{\text{wat}}$				2.02	1.67	1.00
$\text{H}_{\text{wat}}-\text{O}_{\gamma 2}\text{ATP}$	1.72	0.98	1.00			

Table S4. Important bond lengths (Å) of Re, TS and Pr for the model extracted from AceK-ICDH complex.

	associative			dissociative		
	Re	TS	Pr	Re	TS	Pr
$O_{\beta\gamma}ATP-P_{\gamma}ATP$	1.70	1.75	3.54	1.76	2.57	3.93
$O_{wat}-P_{\gamma}ATP$	3.13	2.23	1.61	5.00	2.32	1.72
$O_{\gamma3}ATP-H_{Asp477}$	1.67	1.79	1.65	1.82	1.84	1.70
$O_{Asp457}-H_{wat}$				1.61	1.44	1.00
$H_{wat}-O_{\gamma2}ATP$	1.93	1.01	1.00			

Table S5. Mulliken charges of P_γ and O_{wat} (or O_{Ser113}) of Re, TS and Pr for the ATPase model and the kinase model. The ATPase model corresponds to the Model_{1-wat} of AceK. The kinase model corresponds to the model which has the lowest energy barrier without artificial treatments.⁷

	ATPase Model		Kinase Model	
	P_γ	O_{wat}	P_γ	O_{Ser113}
Re	1.362	-0.865	1.320	-0.691
TS	1.385	-0.818	1.347	-0.709
Pr	1.255	-0.727	1.338	-0.601

References

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Cartesian coordinates of reactants, transition structures and products

1. Model_{1-wat} for AceK

associative Re (-4127.167015 A.U.)

C	42.519517000	28.444285000	55.153726000
O	43.415496000	27.749190000	55.634056000
N	41.396187000	27.892956000	54.598171000
H	40.687025000	28.485622000	54.158481000
C	42.363425000	25.930789000	53.342034000
O	42.601746000	24.728287000	53.263215000
N	42.947081000	26.858892000	52.525284000
H	42.637327000	27.829188000	52.531477000
C	44.678150000	27.553674000	50.814287000
O	44.733678000	27.700384000	49.592984000
N	45.454766000	28.279634000	51.672820000
H	45.127984000	28.307454000	52.632056000
C	49.409313000	32.463485000	48.492978000
H	50.029167000	32.312664000	47.597382000
H	49.600798000	31.598567000	49.143502000
C	47.929173000	32.472816000	48.085757000
H	47.314422000	32.613588000	48.986899000
H	47.732863000	33.350656000	47.452259000
C	47.487876000	31.208379000	47.329522000
H	48.091927000	31.112717000	46.415930000
H	47.695072000	30.312987000	47.932904000
C	46.003947000	31.218791000	46.929712000
H	45.786199000	32.152131000	46.393075000
H	45.791262000	30.399092000	46.236287000
N	45.056122000	31.107651000	48.062473000
H	45.493764000	31.439437000	48.922211000
H	43.846453000	32.167346000	48.080285000
H	44.799243000	30.136000000	48.251016000
C	32.408721000	32.004417000	50.575159000
H	31.655257000	32.803672000	50.649206000
H	32.150727000	31.266031000	51.341841000
C	33.766989000	32.639499000	50.966506000
O	34.402684000	33.245175000	50.057719000
O	34.105656000	32.526819000	52.182422000
C	37.238382000	36.643442000	55.419963000
H	38.159352000	36.622228000	54.821492000

H	37.560798000	36.518638000	56.464039000
C	36.368017000	35.429710000	55.032474000
H	35.450462000	35.428459000	55.639372000
H	36.040152000	35.514305000	53.987936000
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H	38.043529000	34.094444000	54.648233000
H	37.461421000	34.082415000	56.297351000
C	36.352331000	32.795685000	55.013277000
H	36.795034000	32.007509000	55.628895000
H	35.300342000	32.888705000	55.300729000
N	36.378494000	32.279274000	53.608967000
H	36.269157000	31.228244000	53.620741000
H	35.587803000	32.625921000	52.983903000
H	37.306469000	32.415023000	53.162055000
C	36.899009000	36.015765000	50.706154000
H	35.828774000	35.816150000	50.825939000
H	37.039799000	36.336638000	49.664392000
C	37.674038000	34.723198000	50.893805000
O	38.891418000	34.791773000	51.219487000
N	37.021594000	33.586511000	50.696755000
H	37.527319000	32.717834000	50.856164000
H	35.993234000	33.528441000	50.460128000
C	39.079275000	32.979181000	47.332596000
H	38.062133000	32.942237000	46.927618000
H	39.710859000	32.429279000	46.620735000
C	39.090238000	32.194751000	48.633138000
O	38.347064000	31.127599000	48.642235000
O	39.774988000	32.579097000	49.589521000
Mg	40.258979000	33.307277000	51.494155000
O	39.003340000	31.972151000	52.321664000
P	39.123423000	30.438687000	52.015155000
O	38.135828000	30.027239000	50.918319000
O	39.177326000	29.572150000	53.263852000
O	40.628438000	30.240466000	51.231321000
P	42.049883000	30.815342000	51.672633000
O	41.847236000	32.086371000	52.492889000
O	43.013213000	29.756385000	52.087127000
O	42.601001000	31.421793000	50.182636000
P	42.972933000	32.950327000	49.885746000
O	42.023338000	33.978850000	50.437038000
O	43.205885000	32.962090000	48.335234000
O	44.478208000	33.157311000	50.468039000
O	36.452105000	29.499671000	53.544529000
H	37.435963000	29.388232000	53.639378000

H	36.347594000	29.354449000	52.587064000
C	44.692031000	33.631702000	51.807662000
H	44.190153000	32.989766000	52.535199000
H	45.771849000	33.610589000	51.968952000
H	44.328663000	34.659887000	51.904247000
C	49.850251000	33.747978000	49.207008000
H	49.270760000	33.910186000	50.124124000
H	50.909703000	33.706503000	49.484970000
H	49.706386000	34.626757000	48.566340000
C	32.345687000	31.385022000	49.167322000
H	33.026391000	30.529938000	49.081664000
H	31.331834000	31.036077000	48.934200000
H	32.648811000	32.122764000	48.418522000
C	36.569664000	38.022176000	55.269582000
H	35.675931000	38.100065000	55.901605000
H	37.258800000	38.821958000	55.564139000
H	36.260354000	38.209971000	54.235741000
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H	38.450893000	37.326714000	51.473660000
H	36.818815000	38.030222000	51.518740000
H	37.299649000	36.797509000	52.697951000
C	39.582545000	34.418875000	47.496518000
H	40.604474000	34.431940000	47.881729000
H	39.562217000	34.938052000	46.531401000
H	38.956835000	34.976539000	48.199449000
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H	43.412505000	30.220629000	54.384059000
C	43.814138000	26.437073000	51.432890000
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H	43.237041000	26.019401000	50.599731000
C	46.133429000	29.475693000	51.183536000
H	46.601797000	29.240583000	50.226214000
H	45.427553000	30.305775000	51.055964000
H	46.906750000	29.765978000	51.901583000
O	41.001932000	34.447503000	53.195921000
H	41.553002000	33.664320000	53.413713000
H	41.608471000	35.061399000	52.750196000
H	38.326809000	30.649128000	49.590779000

associative TS (-4127.125624 A.U.)

C	42.458249000	28.453433000	55.253063000
O	43.246892000	27.773795000	55.904047000
N	41.395838000	27.893148000	54.587250000
H	40.789300000	28.478555000	54.019702000
C	42.355345000	25.903629000	53.347982000
O	42.589616000	24.699279000	53.305584000
N	42.917671000	26.826202000	52.511409000
H	42.558245000	27.777376000	52.519417000
C	45.101529000	27.247899000	51.201110000
O	46.064159000	26.702255000	50.660652000
N	45.068048000	28.563818000	51.533591000
H	44.185715000	28.979377000	51.828253000
C	49.280085000	33.131248000	47.925829000
H	49.678421000	33.664788000	47.050988000
H	49.622951000	32.091369000	47.832292000
C	47.747824000	33.167615000	47.886255000
H	47.364956000	32.632954000	48.767956000
H	47.408066000	34.208533000	47.993112000
C	47.143370000	32.574768000	46.605857000
H	47.553719000	33.105539000	45.734843000
H	47.445844000	31.522862000	46.498024000
C	45.612673000	32.678752000	46.550246000
H	45.310922000	33.723222000	46.698076000
H	45.243466000	32.380056000	45.563306000
N	44.884108000	31.871861000	47.550690000
H	45.315962000	31.961692000	48.471006000
H	43.474521000	32.527481000	47.950386000
H	44.900719000	30.881030000	47.312805000
C	32.123375000	32.265033000	50.408354000
H	31.432563000	33.080553000	50.148905000
H	31.664244000	31.692318000	51.220968000
C	33.428095000	32.905380000	50.931090000
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C	36.128549000	35.471905000	55.093945000
H	35.115064000	35.630654000	55.490865000
H	36.034261000	35.516095000	54.000636000
C	36.630524000	34.083017000	55.524040000
H	37.681269000	33.960043000	55.222898000
H	36.626445000	34.033042000	56.622277000
C	35.833097000	32.878596000	55.002772000

H	36.137034000	31.983623000	55.556935000
H	34.758688000	33.016175000	55.164272000
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H	36.284917000	31.468827000	53.362027000
H	35.204270000	32.837862000	52.960527000
H	36.879487000	33.038470000	53.192133000
C	36.709025000	36.046919000	50.799354000
H	35.655648000	35.904062000	51.066195000
H	36.712364000	36.348131000	49.742652000
C	37.430156000	34.716472000	50.909722000
O	38.629277000	34.722750000	51.302059000
N	36.751086000	33.625079000	50.593430000
H	37.212274000	32.726705000	50.706151000
H	35.710520000	33.636092000	50.388511000
C	39.392585000	32.916754000	47.257756000
H	38.585366000	32.706425000	46.548638000
H	40.309237000	32.486376000	46.831833000
C	39.116862000	32.157856000	48.540517000
O	38.475034000	31.031872000	48.396030000
O	39.498720000	32.602886000	49.626965000
Mg	39.960132000	33.245801000	51.587599000
O	38.668235000	31.894772000	52.324155000
P	38.615366000	30.419442000	51.888404000
O	37.820387000	30.015622000	50.658118000
O	38.999142000	29.316383000	53.028801000
O	40.229335000	30.223682000	51.155929000
P	41.624620000	30.761939000	51.641923000
O	41.465814000	31.998232000	52.518374000
O	42.581165000	29.685131000	52.048169000
O	42.262392000	31.417114000	50.188597000
P	42.626370000	32.951652000	49.927319000
O	41.742069000	33.959835000	50.607110000
O	42.711315000	33.099597000	48.366357000
O	44.186580000	33.105784000	50.357091000
O	36.759926000	30.209436000	53.088314000
H	38.130750000	29.271184000	53.511371000
H	36.166926000	29.803656000	52.436566000
C	44.555668000	33.088276000	51.748444000
H	44.333154000	32.117630000	52.198775000
H	45.630725000	33.276545000	51.779588000
H	44.026925000	33.876116000	52.291748000
C	49.850251000	33.747978000	49.207008000
H	49.495954000	33.211905000	50.095842000
H	50.945698000	33.715072000	49.214390000

H	49.546951000	34.797096000	49.310251000
C	32.345687000	31.385022000	49.167322000
H	32.992582000	30.530709000	49.400545000
H	31.397393000	30.992459000	48.778273000
H	32.835519000	31.968416000	48.382309000
C	36.569664000	38.022176000	55.269582000
H	35.606598000	38.222621000	55.756338000
H	37.286544000	38.770061000	55.628562000
H	36.433982000	38.177846000	54.194605000
C	37.395899000	37.108534000	51.657100000
H	38.410019000	37.301095000	51.298044000
H	36.833756000	38.049608000	51.628197000
H	37.476226000	36.786115000	52.696975000
C	39.582545000	34.418876000	47.496518000
H	40.396662000	34.598464000	48.199920000
H	39.815264000	34.925033000	46.552494000
H	38.671079000	34.867024000	47.906017000
C	41.338949000	26.451052000	54.389958000
H	41.556147000	25.937691000	55.328110000
H	40.331869000	26.177428000	54.061556000
C	42.637650000	29.961512000	55.106257000
H	41.731820000	30.482830000	54.789085000
H	42.986585000	30.360642000	56.063233000
H	43.403795000	30.139183000	54.348719000
C	43.814138000	26.437074000	51.432889000
H	44.116521000	25.406198000	51.621556000
H	43.279107000	26.440959000	50.469556000
C	46.133430000	29.475693000	51.183536000
H	46.943065000	28.895141000	50.735979000
H	45.786830000	30.229686000	50.460990000
H	46.516912000	30.001457000	52.067840000
O	40.675342000	34.349814000	53.333925000
H	41.240255000	33.573019000	53.531844000
H	41.269198000	34.987166000	52.904064000
H	38.285804000	30.582041000	49.318877000
<u>associative Pr (-4127.19190 A.U.)</u>			
C	42.420653000	28.464133000	55.316830000
O	43.121765000	27.803200000	56.074436000
N	41.398659000	27.897378000	54.584688000
H	40.950943000	28.478715000	53.885741000
C	42.321705000	25.898827000	53.320528000
O	42.500863000	24.686349000	53.238663000
N	42.924700000	26.823403000	52.519500000
H	42.611284000	27.791033000	52.544228000

C	45.103734000	27.260561000	51.235092000
O	46.122998000	26.712176000	50.813815000
N	45.022473000	28.594042000	51.467359000
H	44.113635000	29.028712000	51.676163000
C	48.902863000	32.801802000	48.454345000
H	49.139288000	32.832435000	47.380810000
H	49.095507000	31.768532000	48.775597000
C	47.405917000	33.109392000	48.642127000
H	47.161281000	33.077239000	49.713490000
H	47.192679000	34.136678000	48.313781000
C	46.517779000	32.125325000	47.860433000
H	46.779593000	32.177407000	46.794732000
H	46.748372000	31.096292000	48.172968000
C	45.001684000	32.336949000	47.958123000
H	44.719141000	33.344590000	47.638154000
H	44.492606000	31.623502000	47.303222000
N	44.461057000	32.150733000	49.337704000
H	45.101647000	31.615199000	49.926351000
H	44.229370000	33.069519000	49.830142000
H	43.503914000	31.635084000	49.402649000
C	31.908660000	32.285249000	50.336084000
H	31.158560000	33.002172000	49.975143000
H	31.450930000	31.695695000	51.137360000
C	33.096679000	33.083416000	50.906982000
O	33.713756000	33.821566000	50.095985000
O	33.357431000	32.909333000	52.140371000
C	36.984174000	36.558782000	55.489843000
H	37.955385000	36.379397000	55.008982000
H	37.147863000	36.393244000	56.564851000
C	35.979297000	35.507659000	54.979801000
H	34.993540000	35.688601000	55.433967000
H	35.843527000	35.620236000	53.896207000
C	36.446702000	34.081686000	55.319483000
H	37.429664000	33.885557000	54.871300000
H	36.599155000	34.025873000	56.406761000
C	35.498331000	32.926586000	54.970224000
H	35.794915000	32.044255000	55.544752000
H	34.460255000	33.161276000	55.227104000
N	35.507039000	32.517422000	53.527776000
H	35.309001000	31.512495000	53.437876000
H	34.734571000	32.963570000	52.908172000
H	36.443155000	32.581328000	53.080607000
C	36.511601000	36.094957000	50.941141000
H	35.505386000	36.036908000	51.377159000

H	36.355285000	36.379442000	49.892807000
C	37.121645000	34.703951000	50.967941000
O	38.238733000	34.537973000	51.516748000
N	36.420864000	33.732430000	50.389752000
H	36.784568000	32.789020000	50.481218000
H	35.403718000	33.848958000	50.190734000
C	39.830987000	32.907374000	47.384202000
H	39.469929000	32.498018000	46.436426000
H	40.905698000	32.695008000	47.455424000
C	39.184336000	32.164761000	48.529030000
O	38.557205000	31.063091000	48.204677000
O	39.240724000	32.613867000	49.674032000
Mg	39.447415000	32.898501000	51.687213000
O	37.750831000	31.738367000	52.100192000
P	37.534220000	30.277795000	51.669335000
O	37.236894000	30.030077000	50.207241000
O	38.727176000	29.389503000	52.262554000
O	42.112280000	31.080650000	49.868439000
P	41.987542000	30.919634000	51.383084000
O	40.566049000	31.223972000	51.955977000
O	42.549740000	29.656803000	52.011332000
O	42.949772000	32.172341000	52.028712000
P	42.689734000	33.769980000	51.788702000
O	41.194215000	34.054315000	51.958850000
O	43.400639000	34.254059000	50.550609000
O	43.509324000	34.397235000	53.049133000
O	36.226816000	29.761853000	52.534893000
H	39.564270000	29.943710000	52.158350000
H	35.684759000	29.208983000	51.948712000
C	43.138851000	34.080988000	54.386315000
H	43.071907000	32.997550000	54.535782000
H	43.920966000	34.483657000	55.035816000
H	42.184806000	34.551773000	54.656894000
C	49.850251000	33.747978000	49.207008000
H	49.671093000	33.712048000	50.288270000
H	50.897074000	33.475616000	49.031842000
H	49.714729000	34.787351000	48.883622000
C	32.345687000	31.385022000	49.167322000
H	33.076680000	30.636475000	49.496586000
H	31.492221000	30.851766000	48.730606000
H	32.817769000	31.991503000	48.389099000
C	36.569664000	38.022176000	55.269582000
H	35.629404000	38.249792000	55.787888000
H	37.336152000	38.706042000	55.651687000

H	36.424498000	38.242845000	54.206973000
C	37.395899000	37.108534000	51.657100000
H	38.364800000	37.202373000	51.158591000
H	36.917741000	38.095268000	51.669686000
H	37.596293000	36.804287000	52.685757000
C	39.582545000	34.418876000	47.496518000
H	39.965635000	34.797863000	48.447055000
H	40.083905000	34.950989000	46.680436000
H	38.511877000	34.645419000	47.442749000
C	41.338949000	26.451054000	54.389958000
H	41.591101000	25.960402000	55.330745000
H	40.322564000	26.164159000	54.104262000
C	42.637650000	29.961511000	55.106257000
H	41.689513000	30.500444000	54.996981000
H	43.190367000	30.352856000	55.963061000
H	43.202034000	30.114831000	54.183436000
C	43.814138000	26.437072000	51.432889000
H	44.116631000	25.404156000	51.606336000
H	43.276202000	26.462086000	50.471670000
C	46.133430000	29.475694000	51.183536000
H	47.065981000	29.054225000	51.571411000
H	46.282110000	29.629046000	50.101212000
H	45.950209000	30.437773000	51.673942000
O	39.648940000	33.097853000	53.908721000
H	40.043798000	32.205819000	53.920714000
H	40.399118000	33.676475000	53.649618000
H	38.108570000	30.640156000	49.021732000

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C	42.468266000	28.449641000	55.239366000
O	43.269490000	27.764922000	55.873295000
N	41.401305000	27.894567000	54.578622000
H	40.769960000	28.483487000	54.030245000
C	42.365065000	25.913695000	53.354231000
O	42.627249000	24.715226000	53.315810000
N	42.916192000	26.838569000	52.505684000
H	42.538053000	27.780684000	52.508331000
C	45.059850000	27.285653000	51.125663000
O	45.930072000	26.813532000	50.392636000
N	45.120079000	28.542665000	51.631703000
H	44.275701000	28.964688000	52.010524000
C	49.184731000	32.806204000	48.197432000
H	49.647294000	32.940798000	47.209128000
H	49.375432000	31.763049000	48.484615000

C	47.672540000	33.033831000	48.082632000
H	47.221940000	32.883825000	49.075229000
H	47.484198000	34.086399000	47.823264000
C	46.983148000	32.136304000	47.044143000
H	47.448701000	32.302354000	46.062367000
H	47.144495000	31.076878000	47.289386000
C	45.478538000	32.410911000	46.912617000
H	45.319467000	33.483353000	46.741943000
H	45.064466000	31.887653000	46.044790000
N	44.664528000	32.023286000	48.087075000
H	45.186475000	32.155827000	48.953821000
H	43.425966000	32.933919000	48.362052000
H	44.417733000	31.034393000	48.064859000
C	32.616087000	31.139552000	50.657790000
H	31.680582000	31.254956000	51.226004000
H	32.963390000	30.116523000	50.840203000
C	33.646437000	32.118423000	51.257884000
O	33.663087000	33.288506000	50.766209000
O	34.400201000	31.707438000	52.183785000
C	36.359176000	36.652315000	55.938347000
H	37.065619000	36.541424000	56.773598000
H	35.355683000	36.625413000	56.386895000
C	36.504042000	35.451528000	54.986506000
H	35.839279000	35.594246000	54.124113000
H	37.526182000	35.424646000	54.581982000
C	36.153793000	34.105117000	55.645819000
H	36.821065000	33.912170000	56.499878000
H	35.143520000	34.180973000	56.069778000
C	36.138644000	32.896443000	54.703549000
H	35.597465000	32.053509000	55.131008000
H	35.652473000	33.108585000	53.747547000
N	37.512461000	32.357130000	54.390671000
H	38.263976000	33.061057000	54.356319000
H	37.782521000	31.629598000	55.056030000
H	37.576252000	31.877957000	53.442173000
C	36.438378000	36.056182000	51.107604000
H	35.469075000	36.063548000	51.620706000
H	36.216665000	36.247918000	50.049441000
C	37.054502000	34.675932000	51.219902000
O	38.282715000	34.614330000	51.523406000
N	36.298638000	33.621841000	51.008912000
H	36.710697000	32.696121000	51.130807000
H	35.246835000	33.654928000	50.905297000
C	39.584665000	32.924340000	47.165981000

H	38.835220000	32.669163000	46.404976000
H	40.551535000	32.604149000	46.759923000
C	39.307062000	32.091896000	48.399577000
O	39.388427000	30.801796000	48.265728000
O	39.021924000	32.664552000	49.458287000
Mg	39.513245000	33.077767000	51.377513000
O	38.256595000	31.538265000	51.973444000
P	39.188784000	30.285256000	51.786903000
O	39.009307000	29.571375000	50.461442000
O	39.438485000	29.521936000	53.055600000
O	40.639680000	31.312496000	51.471750000
P	42.164890000	31.299925000	51.995762000
O	42.293826000	32.282608000	53.145063000
O	42.753863000	29.932972000	52.020822000
O	42.883925000	32.097077000	50.668330000
P	42.548519000	33.609374000	50.248429000
O	41.240340000	34.116165000	50.790055000
O	42.682916000	33.609866000	48.687231000
O	43.798839000	34.501394000	50.725716000
O	35.920051000	30.039936000	53.810951000
H	36.595023000	29.570777000	53.296826000
H	35.324232000	30.450603000	53.141052000
C	43.929866000	34.883778000	52.112176000
H	43.779224000	34.023543000	52.769412000
H	44.941544000	35.280208000	52.219468000
H	43.201621000	35.666467000	52.346810000
C	49.850241000	33.747972000	49.207004000
H	49.429423000	33.613526000	50.210856000
H	50.928990000	33.565843000	49.271945000
H	49.704812000	34.798121000	48.924836000
C	32.345668000	31.385013000	49.167309000
H	33.250080000	31.212527000	48.571932000
H	31.559822000	30.719620000	48.786247000
H	32.042639000	32.423362000	49.009384000
C	36.569705000	38.022299000	55.269598000
H	35.855901000	38.177798000	54.452524000
H	36.435085000	38.834921000	55.992920000
H	37.578341000	38.112815000	54.849878000
C	37.395932000	37.108519000	51.657054000
H	38.328248000	37.118628000	51.087611000
H	36.944874000	38.106898000	51.599045000
H	37.649342000	36.912331000	52.700381000
C	39.582528000	34.418972000	47.496453000
H	40.341051000	34.650831000	48.243954000

H	39.791992000	35.006074000	46.593937000
H	38.610605000	34.729079000	47.890007000
C	41.339002000	26.451002000	54.389999000
H	41.551159000	25.933946000	55.327540000
H	40.334479000	26.181055000	54.051054000
C	42.637669000	29.961499000	55.106185000
H	41.727872000	30.467631000	54.786230000
H	42.963370000	30.357483000	56.073532000
H	43.417533000	30.163055000	54.373144000
C	43.814001000	26.437003000	51.432999000
H	44.159642000	25.428768000	51.669351000
H	43.270517000	26.361740000	50.478181000
C	46.133657000	29.475758000	51.183400000
H	47.112382000	28.989363000	51.188443000
H	45.948077000	29.835125000	50.157750000
H	46.148637000	30.334662000	51.859834000
O	40.059701000	33.577190000	53.429434000
H	40.949416000	33.087653000	53.484211000
H	40.288156000	34.514957000	53.327762000
H	39.205951000	30.309468000	49.186318000
<u>dissociative TS (-4127.138570 A.U.)</u>			
C	42.456252000	28.454174000	55.255415000
O	43.240577000	27.769264000	55.909590000
N	41.398423000	27.894799000	54.579824000
H	40.773347000	28.479573000	54.025961000
C	42.339730000	25.908642000	53.334048000
O	42.572699000	24.703760000	53.279251000
N	42.900172000	26.832328000	52.496099000
H	42.556807000	27.788456000	52.522310000
C	45.089943000	27.271756000	51.218897000
O	46.094578000	26.736321000	50.746238000
N	45.023447000	28.597434000	51.486389000
H	44.137817000	29.043460000	51.735064000
C	49.219142000	32.684254000	48.302405000
H	49.708380000	32.700199000	47.317950000
H	49.405683000	31.685751000	48.720949000
C	47.710409000	32.887109000	48.121702000
H	47.239571000	32.874832000	49.116045000
H	47.527556000	33.892895000	47.714266000
C	47.042210000	31.850555000	47.206779000
H	47.539382000	31.862834000	46.226311000
H	47.181926000	30.839225000	47.614515000
C	45.545610000	32.116817000	46.989804000
H	45.411821000	33.143438000	46.624458000

H	45.143761000	31.452290000	46.217989000
N	44.699921000	31.957517000	48.191525000
H	45.198898000	32.260326000	49.028114000
H	43.403770000	32.895584000	48.346332000
H	44.459773000	30.980913000	48.358396000
C	32.791497000	30.904043000	50.553956000
H	31.908868000	30.749197000	51.192690000
H	33.300330000	29.934797000	50.497824000
C	33.715142000	31.904155000	51.280877000
O	33.524719000	33.131188000	51.044158000
O	34.596406000	31.440412000	52.067335000
C	36.338939000	36.660271000	55.949220000
H	37.018636000	36.563101000	56.807971000
H	35.321564000	36.636795000	56.365415000
C	36.519730000	35.444767000	55.021321000
H	35.867660000	35.556656000	54.145078000
H	37.549644000	35.431022000	54.636682000
C	36.186749000	34.106483000	55.706930000
H	36.835064000	33.956399000	56.583403000
H	35.161674000	34.159627000	56.097205000
C	36.245006000	32.871345000	54.799642000
H	35.763711000	32.014833000	55.277797000
H	35.727395000	33.021961000	53.847921000
N	37.644319000	32.428509000	54.470203000
H	38.336004000	33.184744000	54.326544000
H	38.033290000	31.801284000	55.177732000
H	37.704732000	31.909563000	53.518905000
C	36.416790000	36.074742000	51.113154000
H	35.436826000	36.131490000	51.601898000
H	36.232883000	36.245867000	50.043818000
C	36.987484000	34.679593000	51.271126000
O	38.230431000	34.574709000	51.463050000
N	36.168813000	33.650200000	51.215732000
H	36.549077000	32.710959000	51.333827000
H	35.125665000	33.696898000	51.155414000
C	39.598197000	32.916189000	47.198036000
H	38.943208000	32.655655000	46.355575000
H	40.603105000	32.579620000	46.918995000
C	39.167136000	32.100454000	48.397912000
O	39.264999000	30.802763000	48.275676000
O	38.753797000	32.663547000	49.416332000
Mg	39.445137000	32.981790000	51.322629000
O	38.078113000	31.568365000	52.061482000
P	38.676184000	30.139264000	51.854473000

O	38.555451000	29.550208000	50.473059000
O	39.197748000	29.444888000	53.065371000
O	40.523286000	31.264439000	51.311783000
P	41.967258000	31.230341000	51.908075000
O	42.102580000	32.187807000	53.097056000
O	42.608832000	29.877890000	51.963371000
O	42.847476000	32.068475000	50.654676000
P	42.482817000	33.548906000	50.201198000
O	41.147594000	34.054144000	50.683001000
O	42.651532000	33.556080000	48.635753000
O	43.702871000	34.482111000	50.694658000
O	36.361947000	29.337145000	52.154625000
H	36.421879000	28.963698000	51.261630000
H	35.691851000	30.069168000	52.081138000
C	43.842737000	34.771097000	52.101497000
H	43.644892000	33.882348000	52.707918000
H	44.871122000	35.111577000	52.241796000
H	43.151769000	35.573742000	52.380526000
C	49.850241000	33.747972000	49.207004000
H	49.404705000	33.729907000	50.209038000
H	50.928749000	33.588709000	49.320193000
H	49.702245000	34.754921000	48.797283000
C	32.345668000	31.385013000	49.167309000
H	33.203700000	31.480913000	48.491346000
H	31.632381000	30.687303000	48.709717000
H	31.880363000	32.371021000	49.246640000
C	36.569705000	38.022299000	55.269598000
H	35.882025000	38.167449000	54.428713000
H	36.411448000	38.842606000	55.979073000
H	37.591315000	38.108276000	54.881811000
C	37.395932000	37.108518000	51.657054000
H	38.341391000	37.066430000	51.112100000
H	36.984188000	38.120714000	51.560492000
H	37.615914000	36.933802000	52.712435000
C	39.582528000	34.418972000	47.496453000
H	40.237435000	34.651585000	48.335673000
H	39.925414000	34.979141000	46.618648000
H	38.572786000	34.756726000	47.748200000
C	41.339000000	26.451002000	54.390003000
H	41.574581000	25.940505000	55.325410000
H	40.327463000	26.175264000	54.077582000
C	42.637669000	29.961499000	55.106184000
H	41.715636000	30.484957000	54.854627000
H	43.053117000	30.353397000	56.039405000

H	43.345469000	30.147897000	54.298242000
C	43.814013000	26.437015000	51.432993000
H	44.130327000	25.415232000	51.644939000
H	43.290644000	26.416314000	50.463305000
C	46.133648000	29.475746000	51.183403000
H	47.054530000	29.116461000	51.654923000
H	46.328267000	29.539577000	50.101168000
H	45.897503000	30.472772000	51.565026000
O	40.000401000	33.566986000	53.353586000
H	40.884649000	33.017833000	53.381903000
H	40.270937000	34.481997000	53.176314000
H	38.995696000	30.338388000	49.153202000
<u>dissociative Pr (-4127.182066 A.U.)</u>			
C	42.541943000	28.441172000	55.123440000
O	43.470512000	27.741304000	55.529385000
N	41.402585000	27.893119000	54.596952000
H	40.619792000	28.490904000	54.303054000
C	42.419341000	25.940982000	53.397908000
O	42.775987000	24.769149000	53.418074000
N	42.919927000	26.860588000	52.503175000
H	42.416006000	27.735085000	52.408162000
C	44.831276000	27.427536000	50.877194000
O	45.310330000	27.211716000	49.764071000
N	45.181714000	28.480223000	51.651951000
H	44.777380000	28.562262000	52.575846000
C	48.812193000	32.776414000	48.638225000
H	49.113574000	32.450137000	47.633037000
H	48.776962000	31.870854000	49.258598000
C	47.415040000	33.402463000	48.579640000
H	47.186869000	33.788619000	49.583363000
H	47.436173000	34.274534000	47.907288000
C	46.310658000	32.433220000	48.135963000
H	46.564296000	31.996890000	47.160935000
H	46.243526000	31.598776000	48.845201000
C	44.935131000	33.094405000	48.010255000
H	44.930210000	33.857661000	47.224374000
H	44.163046000	32.358066000	47.773095000
N	44.529889000	33.750771000	49.281012000
H	45.203929000	34.465590000	49.560421000
H	43.596582000	34.278004000	49.243276000
H	44.482547000	33.068985000	50.105552000
C	33.569777000	30.835157000	49.915856000
H	33.386468000	29.818112000	50.286086000
H	34.436955000	30.757319000	49.244297000

C	33.972672000	31.710810000	51.093770000
O	33.497204000	32.814392000	51.290031000
O	34.867069000	31.233583000	51.974825000
C	37.276557000	37.140512000	56.309882000
H	38.318292000	37.475780000	56.417135000
H	36.808708000	37.289451000	57.294210000
C	37.264247000	35.642103000	55.967488000
H	36.221135000	35.294591000	55.906298000
H	37.701045000	35.497502000	54.971771000
C	38.030322000	34.783373000	56.985726000
H	39.089348000	35.077178000	56.983440000
H	37.649041000	34.990245000	57.996848000
C	37.944124000	33.268501000	56.749677000
H	38.518530000	32.758019000	57.531416000
H	36.896586000	32.941040000	56.861189000
N	38.509435000	32.869470000	55.451338000
H	39.878686000	33.522665000	54.672142000
H	38.675457000	31.862716000	55.398286000
H	37.862411000	33.058593000	54.687976000
C	36.399592000	36.005402000	52.008772000
H	35.792922000	36.286351000	52.880698000
H	35.690270000	35.831343000	51.189863000
C	37.112103000	34.700011000	52.327480000
O	38.337487000	34.703324000	52.552432000
N	36.382503000	33.583305000	52.402611000
H	36.900627000	32.704260000	52.484099000
H	35.398762000	33.552773000	52.157197000
C	39.378596000	32.909181000	47.630160000
H	38.425755000	32.601926000	47.173799000
H	40.151841000	32.353693000	47.084988000
C	39.382143000	32.374190000	49.072110000
O	39.481725000	31.127899000	49.198056000
O	39.261223000	33.228905000	50.005600000
Mg	39.899462000	33.364899000	51.907907000
O	38.660236000	31.833705000	52.609557000
P	38.759116000	30.302707000	52.612109000
O	39.624852000	29.782209000	51.393799000
O	39.131513000	29.601438000	53.897144000
O	41.753011000	32.518538000	51.667384000
P	43.125496000	32.945223000	52.150447000
O	43.203939000	32.926639000	53.756743000
O	44.352600000	32.292612000	51.552880000
O	43.313013000	34.572888000	51.811619000
P	42.192834000	35.499829000	51.027290000

O	40.844963000	35.275787000	51.681458000
O	42.405379000	35.335203000	49.540398000
O	42.749214000	36.983530000	51.411897000
O	37.178323000	29.796904000	52.262493000
H	37.055037000	28.989086000	52.786383000
H	35.500320000	30.533310000	51.690755000
C	42.627716000	37.432382000	52.759572000
H	43.199423000	36.790185000	53.440845000
H	43.036589000	38.446456000	52.793297000
H	41.577580000	37.452653000	53.071456000
C	49.850241000	33.747972000	49.207004000
H	49.587533000	34.050621000	50.227753000
H	50.847766000	33.294948000	49.240761000
H	49.918553000	34.658326000	48.598062000
C	32.345668000	31.385013000	49.167309000
H	32.541882000	32.394573000	48.797299000
H	32.098235000	30.740144000	48.317573000
H	31.476389000	31.438330000	49.829624000
C	36.569705000	38.022299000	55.269598000
H	35.524832000	37.715034000	55.134025000
H	36.567231000	39.074534000	55.578967000
H	37.065828000	37.963172000	54.296669000
C	37.395932000	37.108519000	51.657054000
H	37.973030000	36.841973000	50.767272000
H	36.873189000	38.053627000	51.468799000
H	38.118245000	37.256187000	52.462489000
C	39.582528000	34.418972000	47.496453000
H	40.513502000	34.738241000	47.973865000
H	39.606176000	34.715390000	46.438608000
H	38.769639000	34.965007000	47.985725000
C	41.339001000	26.450997000	54.389998000
H	41.500645000	25.896792000	55.318442000
H	40.349907000	26.202757000	53.993120000
C	42.637670000	29.961503000	55.106185000
H	41.672389000	30.443330000	54.927630000
H	43.063234000	30.304102000	56.053402000
H	43.320950000	30.276106000	54.311333000
C	43.814002000	26.437005000	51.433000000
H	44.356463000	25.565164000	51.813592000
H	43.252669000	26.085604000	50.557291000
C	46.133657000	29.475757000	51.183400000
H	47.117751000	29.341342000	51.653936000
H	46.243061000	29.332401000	50.106846000
H	45.753035000	30.478159000	51.399417000

O	40.615654000	33.789845000	54.027797000
H	42.305473000	33.181543000	54.089900000
H	40.544597000	34.745726000	53.861413000
H	39.576010000	30.382424000	50.554718000

2. Model_{2-wat} for AceK

associative Re (-4203.618278 A.U.)

C	42.499700000	28.445187000	55.208108000
O	43.339057000	27.754615000	55.783898000
N	41.408493000	27.891768000	54.588029000
H	40.746723000	28.502447000	54.106048000
C	42.356796000	25.904462000	53.347653000
O	42.603193000	24.701614000	53.305868000
N	42.908527000	26.826026000	52.502182000
H	42.548700000	27.776013000	52.519380000
C	45.051698000	27.297857000	51.128712000
O	45.939023000	26.828538000	50.412650000
N	45.091679000	28.564359000	51.608613000
H	44.239317000	28.983603000	51.980309000
C	49.355826000	32.802060000	48.107124000
H	49.806055000	33.089086000	47.145992000
H	49.704634000	31.781125000	48.315269000
C	47.828298000	32.798463000	47.966397000
H	47.389639000	32.498937000	48.929370000
H	47.479964000	33.825521000	47.780645000
C	47.313013000	31.887304000	46.842735000
H	47.795029000	32.177343000	45.898010000
H	47.609983000	30.846083000	47.034348000
C	45.792892000	31.960622000	46.639802000
H	45.492632000	33.006416000	46.498612000
H	45.502063000	31.422782000	45.731144000
N	44.973880000	31.419239000	47.744935000
H	45.337824000	31.728892000	48.646824000
H	43.509891000	32.063028000	47.836905000
H	45.002768000	30.400021000	47.765207000
C	32.034842000	32.267241000	50.385725000
H	31.622605000	33.230640000	50.067321000
H	31.295551000	31.762406000	51.019719000
C	33.309879000	32.509920000	51.210232000
O	33.855036000	33.651757000	51.111851000
O	33.722474000	31.525083000	51.887031000
C	37.032857000	36.564577000	55.389591000
H	37.960762000	36.430126000	54.817752000

H	37.289539000	36.337449000	56.433474000
C	35.976148000	35.571908000	54.885506000
H	35.132515000	35.548215000	55.591661000
H	35.560152000	35.950136000	53.940635000
C	36.497080000	34.146813000	54.641739000
H	37.342992000	34.180340000	53.942982000
H	36.885159000	33.708030000	55.570639000
C	35.388769000	33.273823000	54.052071000
H	34.636828000	33.019562000	54.806708000
H	34.873468000	33.794338000	53.238199000
N	35.869186000	31.996413000	53.451329000
H	36.127387000	31.261103000	54.143748000
H	35.089484000	31.671535000	52.793618000
H	36.748381000	32.122960000	52.900164000
C	36.523942000	36.119445000	50.883847000
H	35.580881000	35.905565000	51.400505000
H	36.237063000	36.546370000	49.912456000
C	37.229125000	34.803505000	50.601378000
O	38.489872000	34.748888000	50.650174000
N	36.470507000	33.766481000	50.272378000
H	36.954372000	32.904794000	50.013686000
H	35.451781000	33.746208000	50.481117000
C	40.205824000	33.843669000	46.224087000
H	39.653059000	34.155403000	45.325842000
H	41.233279000	34.196776000	46.084903000
C	40.243982000	32.335343000	46.197458000
O	40.984179000	31.857860000	45.170940000
O	39.664880000	31.576329000	46.952684000
Mg	39.580006000	33.086004000	51.080700000
O	38.425719000	31.973826000	52.345383000
P	39.069512000	30.552015000	52.211824000
O	38.503414000	29.753669000	51.059849000
O	39.423975000	29.878955000	53.521871000
O	40.584922000	31.212799000	51.507360000
P	42.144321000	31.101676000	51.872316000
O	42.537576000	32.252324000	52.771970000
O	42.593820000	29.697492000	52.092343000
O	42.784438000	31.509698000	50.323872000
P	42.581636000	32.915906000	49.611712000
O	41.342367000	33.649258000	50.045540000
O	42.658172000	32.623152000	48.067868000
O	43.931595000	33.765951000	49.852821000
O	37.082336000	29.935989000	54.990498000
H	37.994322000	29.988889000	54.599823000

H	36.773099000	29.071643000	54.678622000
C	44.199706000	34.392995000	51.126824000
H	44.022747000	33.695147000	51.949095000
H	45.246615000	34.701658000	51.094485000
H	43.564023000	35.277594000	51.239193000
C	49.850241000	33.747972000	49.207004000
H	49.444585000	33.463997000	50.185546000
H	50.943388000	33.734048000	49.284091000
H	49.542424000	34.782021000	49.008066000
C	32.345668000	31.385013000	49.167309000
H	32.772327000	30.430803000	49.492535000
H	31.443758000	31.179094000	48.577137000
H	33.073727000	31.873656000	48.508415000
C	36.569702000	38.022293000	55.269587000
H	35.648732000	38.194299000	55.841573000
H	37.328957000	38.717668000	55.647309000
H	36.363949000	38.285271000	54.226333000
C	37.395937000	37.108521000	51.657061000
H	38.296517000	37.357489000	51.088689000
H	36.842973000	38.034225000	51.850710000
H	37.718205000	36.691237000	52.613663000
C	39.582526000	34.418974000	47.496455000
H	40.198789000	34.207565000	48.365157000
H	39.491805000	35.506908000	47.402282000
H	38.581232000	34.014377000	47.667243000
C	41.338994000	26.450996000	54.389999000
H	41.551241000	25.924459000	55.323027000
H	40.331116000	26.186692000	54.055672000
C	42.637680000	29.961507000	55.106182000
H	41.714797000	30.456245000	54.801527000
H	42.955395000	30.341359000	56.083165000
H	43.416899000	30.196109000	54.381860000
C	43.813997000	26.436998000	51.433002000
H	44.172077000	25.431980000	51.665682000
H	43.274608000	26.356670000	50.475527000
C	46.133658000	29.475764000	51.183401000
H	46.084360000	29.691979000	50.104048000
H	46.029220000	30.410663000	51.740286000
H	47.120526000	29.046130000	51.380781000
O	40.556411000	34.062141000	52.704000000
H	41.285722000	33.410607000	52.923825000
H	41.022457000	34.803867000	52.287687000
H	40.932515000	30.885436000	45.240093000
O	38.605278000	31.940025000	49.530612000

H	38.499742000	31.014601000	49.922261000
H	38.976914000	31.838589000	48.629865000
<u>associative TS (-4203.562989 A.U.)</u>			
C	42.489242000	28.449945000	55.236600000
O	43.300166000	27.761950000	55.851305000
N	41.406707000	27.890775000	54.598710000
H	40.808026000	28.504398000	54.056326000
C	42.346044000	25.898152000	53.340411000
O	42.572861000	24.691775000	53.291925000
N	42.908335000	26.819261000	52.504985000
H	42.555867000	27.772288000	52.524407000
C	45.063436000	27.292595000	51.169650000
O	46.018294000	26.792175000	50.571733000
N	45.037555000	28.596084000	51.539049000
H	44.165416000	29.015948000	51.865001000
C	49.399346000	32.865839000	48.037150000
H	49.821799000	33.256587000	47.100203000
H	49.811557000	31.854509000	48.159135000
C	47.873165000	32.778775000	47.902202000
H	47.459841000	32.367262000	48.834543000
H	47.459673000	33.794130000	47.808606000
C	47.409649000	31.940497000	46.701425000
H	47.868875000	32.343575000	45.787134000
H	47.774789000	30.907696000	46.799869000
C	45.886880000	31.929718000	46.499994000
H	45.514879000	32.961052000	46.462574000
H	45.634786000	31.467464000	45.539335000
N	45.105715000	31.226794000	47.538417000
H	45.420167000	31.504570000	48.468749000
H	43.583475000	31.783855000	47.665290000
H	45.233272000	30.217050000	47.477778000
C	32.203042000	32.691405000	49.968964000
H	31.761189000	33.473355000	49.341687000
H	31.540393000	32.516606000	50.825911000
C	33.567095000	33.182120000	50.496091000
O	34.105415000	34.144551000	49.873348000
O	34.039577000	32.547886000	51.482773000
C	37.300509000	36.824356000	55.913688000
H	38.359981000	37.090643000	56.024688000
H	36.921187000	36.675699000	56.935347000
C	37.216033000	35.481419000	55.148367000
H	37.425461000	35.664285000	54.089524000
H	38.033290000	34.834899000	55.486948000
C	35.873899000	34.721141000	55.311504000

H	35.995052000	33.910277000	56.040819000
H	35.120077000	35.397950000	55.738930000
C	35.233280000	34.158143000	54.036638000
H	34.261743000	33.714815000	54.274599000
H	35.040908000	34.963665000	53.318455000
N	35.990312000	33.109113000	53.302743000
H	36.275751000	32.199002000	53.822141000
H	35.385970000	32.841813000	52.471300000
H	36.910388000	33.402970000	52.944418000
C	36.992876000	36.434352000	50.344441000
H	35.905401000	36.372754000	50.236243000
H	37.380783000	37.009890000	49.493311000
C	37.601389000	35.051250000	50.256751000
O	38.843811000	34.933812000	50.475620000
N	36.805536000	34.044044000	49.949898000
H	37.242107000	33.126019000	49.848830000
H	35.754577000	34.130391000	49.914542000
C	40.123408000	33.823038000	46.195179000
H	39.528395000	34.136677000	45.325394000
H	41.147072000	34.159960000	45.993990000
C	40.143833000	32.313536000	46.174761000
O	40.760929000	31.826405000	45.074340000
O	39.651308000	31.560458000	46.994969000
Mg	39.879242000	33.302396000	51.043915000
O	38.605725000	32.598505000	52.462727000
P	38.897478000	31.086919000	52.525381000
O	38.289131000	30.162417000	51.509987000
O	39.495217000	30.488666000	53.880106000
O	40.562127000	31.382275000	51.701857000
P	42.111135000	31.053426000	51.860780000
O	42.791436000	32.180394000	52.613320000
O	42.421070000	29.614321000	52.118012000
O	42.616190000	31.257275000	50.212971000
P	42.690982000	32.646890000	49.458346000
O	41.601532000	33.605732000	49.858012000
O	42.720580000	32.303829000	47.921308000
O	44.173302000	33.258983000	49.668869000
O	37.150317000	30.885044000	54.090031000
H	38.561998000	30.488010000	54.378412000
H	36.676768000	30.112408000	53.743178000
C	44.533516000	34.030407000	50.835056000
H	44.320782000	33.466628000	51.745725000
H	45.602258000	34.233184000	50.738155000
H	43.985156000	34.978501000	50.832322000

C	49.850241000	33.747972000	49.207004000
H	49.470281000	33.364787000	50.161837000
H	50.943130000	33.789583000	49.277172000
H	49.483505000	34.775579000	49.092584000
C	32.345668000	31.385013000	49.167309000
H	32.800607000	30.608013000	49.790416000
H	31.372079000	31.022129000	48.814486000
H	32.988448000	31.535401000	48.291710000
C	36.569702000	38.022293000	55.269587000
H	35.505005000	37.810982000	55.107108000
H	36.636061000	38.907445000	55.913123000
H	37.009191000	38.277348000	54.299799000
C	37.395937000	37.108520000	51.657060000
H	38.475995000	37.045869000	51.809534000
H	37.100176000	38.164437000	51.661034000
H	36.898123000	36.627192000	52.500049000
C	39.582526000	34.418974000	47.496457000
H	40.246266000	34.200109000	48.326751000
H	39.512714000	35.507964000	47.399362000
H	38.584354000	34.037504000	47.721606000
C	41.338992000	26.450997000	54.390000000
H	41.560532000	25.930666000	55.323716000
H	40.327566000	26.181879000	54.070387000
C	42.637680000	29.961507000	55.106182000
H	41.714663000	30.463676000	54.816523000
H	42.984407000	30.350530000	56.069379000
H	43.402771000	30.177402000	54.360330000
C	43.813998000	26.436998000	51.433001000
H	44.160207000	25.424297000	51.646326000
H	43.277193000	26.387607000	50.471459000
C	46.133658000	29.475764000	51.183401000
H	46.212314000	29.619342000	50.094190000
H	45.972706000	30.445210000	51.662196000
H	47.085508000	29.056099000	51.523223000
O	41.090039000	34.275634000	52.511340000
H	41.725241000	33.537550000	52.748059000
H	41.634174000	34.893678000	51.999069000
H	40.718368000	30.854726000	45.157253000
O	38.805295000	32.040193000	49.616676000
H	38.596376000	31.185468000	50.087265000
H	39.119220000	31.836763000	48.710661000
<u>associative Pr (-4203.634028 A.U.)</u>			
C	42.363088000	28.477921000	55.366369000
O	42.971462000	27.836963000	56.218335000

N	41.395572000	27.901416000	54.566121000
H	41.095184000	28.467559000	53.777638000
C	42.349914000	25.892717000	53.347652000
O	42.587249000	24.688254000	53.307177000
N	42.915133000	26.815666000	52.512314000
H	42.530014000	27.757847000	52.486539000
C	45.071344000	27.296057000	51.240557000
O	46.127195000	26.775022000	50.880316000
N	44.958859000	28.643056000	51.399526000
H	44.061411000	29.072327000	51.630109000
C	49.282327000	32.605999000	48.357964000
H	49.774494000	32.597452000	47.375108000
H	49.522425000	31.642641000	48.828345000
C	47.765155000	32.712562000	48.163886000
H	47.290861000	32.734948000	49.155908000
H	47.528505000	33.678296000	47.692230000
C	47.161824000	31.581251000	47.320385000
H	47.667957000	31.548146000	46.344816000
H	47.353141000	30.611297000	47.801545000
C	45.654539000	31.742671000	47.071345000
H	45.465395000	32.712244000	46.593251000
H	45.299928000	30.974911000	46.375471000
N	44.799667000	31.671373000	48.270695000
H	45.173316000	32.255391000	49.019333000
H	43.300479000	32.336189000	48.233270000
H	44.756169000	30.723658000	48.645092000
C	32.260420000	32.802876000	49.737292000
H	32.493453000	33.553406000	48.974426000
H	31.230282000	33.007487000	50.066114000
C	33.170644000	33.068742000	50.945118000
O	33.713012000	34.196561000	51.042084000
O	33.289943000	32.126952000	51.808811000
C	37.256424000	36.655473000	55.450175000
H	38.307873000	36.754116000	55.152616000
H	37.272407000	36.386756000	56.516147000
C	36.620263000	35.506110000	54.636895000
H	36.310366000	35.902329000	53.665637000
H	37.381582000	34.744963000	54.425055000
C	35.393315000	34.849612000	55.288704000
H	35.702476000	34.167082000	56.093040000
H	34.770268000	35.619099000	55.766507000
C	34.476975000	34.127567000	54.297257000
H	33.570812000	33.773361000	54.800098000
H	34.160603000	34.792670000	53.489007000

N	35.047181000	32.934502000	53.607935000
H	35.218750000	32.141061000	54.229649000
H	34.316539000	32.598841000	52.859714000
H	35.931302000	33.051511000	53.072510000
C	36.390385000	36.244857000	50.904229000
H	35.531490000	35.966779000	51.528683000
H	35.962013000	36.791307000	50.054894000
C	37.000986000	34.949870000	50.391955000
O	38.171197000	34.642859000	50.699703000
N	36.222113000	34.204093000	49.595658000
H	36.598657000	33.291182000	49.340200000
H	35.213051000	34.293156000	49.724916000
C	40.402904000	33.856255000	46.336068000
H	39.994774000	34.170756000	45.363808000
H	41.436329000	34.213969000	46.366328000
C	40.454065000	32.348680000	46.308372000
O	41.386526000	31.880107000	45.443943000
O	39.741844000	31.578706000	46.926385000
Mg	38.944200000	32.700326000	51.078545000
O	37.172274000	32.052311000	51.926159000
P	36.644779000	30.632999000	51.573601000
O	36.347014000	30.431494000	50.100841000
O	37.659587000	29.557895000	52.205780000
O	39.933402000	30.905859000	51.399146000
P	41.405342000	30.862151000	51.883433000
O	41.688340000	31.934528000	52.936494000
O	42.006800000	29.486802000	52.063466000
O	42.308471000	31.433214000	50.487893000
P	42.137851000	32.917476000	49.973816000
O	40.820785000	33.551457000	50.321711000
O	42.433045000	32.861262000	48.420058000
O	43.412598000	33.768465000	50.496625000
O	35.320870000	30.329026000	52.467885000
H	38.583855000	29.864447000	52.006948000
H	34.528179000	30.666284000	51.991594000
C	43.466197000	34.259391000	51.853115000
H	43.202571000	33.469360000	52.560867000
H	44.491791000	34.603041000	52.008441000
H	42.780088000	35.106035000	51.963776000
C	49.850241000	33.747972000	49.207004000
H	49.402565000	33.756994000	50.208073000
H	50.935390000	33.654776000	49.329359000
H	49.648817000	34.722747000	48.745980000
C	32.345668000	31.385013000	49.167309000

H	32.041844000	30.650828000	49.919312000
H	31.695868000	31.273869000	48.290833000
H	33.371242000	31.137770000	48.870739000
C	36.569702000	38.022292000	55.269587000
H	35.506669000	37.981527000	55.540171000
H	37.039839000	38.784509000	55.902083000
H	36.634557000	38.360810000	54.231253000
C	37.395937000	37.108521000	51.657062000
H	38.173576000	37.474536000	50.977387000
H	36.900830000	37.979751000	52.098549000
H	37.901088000	36.547628000	52.443360000
C	39.582526000	34.418974000	47.496454000
H	39.998527000	34.138437000	48.460038000
H	39.571582000	35.513649000	47.436148000
H	38.546281000	34.072959000	47.454960000
C	41.338990000	26.451002000	54.390006000
H	41.572562000	25.975688000	55.343002000
H	40.330144000	26.154546000	54.084902000
C	42.637679000	29.961503000	55.106182000
H	41.754265000	30.528776000	54.817422000
H	43.084589000	30.384787000	56.009596000
H	43.347830000	30.049564000	54.280434000
C	43.814001000	26.436995000	51.432995000
H	44.149850000	25.417372000	51.623458000
H	43.278341000	26.430739000	50.469386000
C	46.133660000	29.475765000	51.183402000
H	46.479880000	29.421831000	50.142100000
H	45.879024000	30.509661000	51.431354000
H	46.963081000	29.145657000	51.817591000
O	39.631311000	33.572909000	52.905879000
H	40.423935000	32.966694000	53.076299000
H	40.023462000	34.383960000	52.545101000
H	41.326065000	30.907439000	45.500327000
O	38.163328000	32.069529000	49.206435000
H	37.525279000	31.305553000	49.369296000
H	38.737385000	31.856251000	48.442603000

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C	42.579779000	28.439867000	55.101771000
O	43.527169000	27.750816000	55.487994000
N	41.424512000	27.884679000	54.624251000
H	40.713004000	28.510317000	54.238139000
C	42.362907000	25.920134000	53.343306000
O	42.629329000	24.720929000	53.293084000

N	42.905916000	26.840638000	52.495315000
H	42.580454000	27.806857000	52.499289000
C	44.667297000	27.565023000	50.823916000
O	44.761903000	27.693226000	49.600031000
N	45.399911000	28.321476000	51.688492000
H	45.060104000	28.363220000	52.643316000
C	49.420575000	32.424895000	48.554233000
H	50.034031000	32.248797000	47.658709000
H	49.638955000	31.592891000	49.238226000
C	47.935714000	32.375518000	48.157931000
H	47.319735000	32.509322000	49.059418000
H	47.705808000	33.232481000	47.507288000
C	47.541055000	31.078786000	47.427484000
H	48.174183000	30.974662000	46.534455000
H	47.756546000	30.206549000	48.060891000
C	46.070147000	31.027744000	46.975324000
H	45.830239000	31.951231000	46.431762000
H	45.922720000	30.200663000	46.273259000
N	45.072511000	30.867542000	48.055348000
H	45.379767000	31.369497000	48.888580000
H	43.676677000	31.640484000	47.883564000
H	44.972866000	29.890044000	48.347208000
C	32.355826000	32.709192000	49.944598000
H	31.762938000	33.468166000	49.423471000
H	31.908250000	32.546687000	50.934820000
C	33.788462000	33.240147000	50.143269000
O	34.086309000	34.330665000	49.576351000
O	34.575794000	32.538962000	50.843907000
C	37.016938000	36.722358000	55.966838000
H	38.010945000	36.888684000	56.402102000
H	36.347520000	36.518598000	56.815815000
C	37.088500000	35.465928000	55.069921000
H	37.671666000	35.691589000	54.169442000
H	37.657210000	34.691424000	55.601778000
C	35.708799000	34.905348000	54.679647000
H	35.212703000	34.508334000	55.579264000
H	35.064040000	35.720995000	54.325787000
C	35.675362000	33.845566000	53.573421000
H	34.646372000	33.541756000	53.369137000
H	36.068928000	34.222729000	52.628464000
N	36.446071000	32.595971000	53.872560000
H	36.060974000	31.759549000	53.286418000
H	37.459469000	32.630429000	53.562820000
H	36.404775000	32.339232000	54.860659000

C	37.133525000	36.522604000	50.269592000
H	36.071196000	36.563665000	50.009171000
H	37.686464000	37.094157000	49.512287000
C	37.629925000	35.093386000	50.205526000
O	38.811653000	34.859204000	50.598630000
N	36.805313000	34.176069000	49.742820000
H	37.147581000	33.213614000	49.721651000
H	35.771181000	34.335396000	49.631530000
C	40.244620000	33.740364000	46.295640000
H	39.748046000	34.008672000	45.352286000
H	41.289530000	34.052655000	46.183550000
C	40.247700000	32.231712000	46.363121000
O	40.925052000	31.678609000	45.332867000
O	39.697449000	31.531466000	47.193388000
Mg	39.789076000	33.169513000	51.113852000
O	38.836042000	32.263685000	52.677799000
P	39.233072000	30.748872000	52.506046000
O	38.316922000	30.066158000	51.487182000
O	39.649697000	30.026789000	53.750832000
O	40.668898000	31.103482000	51.519401000
P	42.248857000	31.002226000	51.877348000
O	42.652239000	32.195646000	52.719692000
O	42.735859000	29.624034000	52.144683000
O	42.857277000	31.335517000	50.306349000
P	42.716206000	32.697974000	49.507793000
O	41.485336000	33.484960000	49.865678000
O	42.857534000	32.295687000	47.995540000
O	44.080316000	33.533693000	49.746883000
O	35.647990000	30.580724000	52.334750000
H	36.513414000	30.301456000	51.943773000
H	35.179859000	31.114852000	51.644169000
C	44.323084000	34.247009000	50.975619000
H	44.112392000	33.614478000	51.842045000
H	45.376298000	34.535764000	50.953435000
H	43.706311000	35.152539000	51.004053000
C	49.850241000	33.747972000	49.207004000
H	49.281995000	33.941425000	50.125099000
H	50.913891000	33.731987000	49.470569000
H	49.684989000	34.595739000	48.530680000
C	32.345668000	31.385014000	49.167308000
H	32.953112000	30.637184000	49.686807000
H	31.328027000	30.989289000	49.057602000
H	32.764013000	31.518705000	48.162200000
C	36.569706000	38.022298000	55.269595000

H	35.569309000	37.932317000	54.830273000
H	36.540921000	38.852334000	55.985142000
H	37.261738000	38.295623000	54.465189000
C	37.395932000	37.108521000	51.657053000
H	38.441237000	36.967216000	51.942294000
H	37.165953000	38.180384000	51.681140000
H	36.764633000	36.622192000	52.404992000
C	39.582529000	34.418979000	47.496449000
H	40.160726000	34.256796000	48.400495000
H	39.524797000	35.499031000	47.317467000
H	38.565121000	34.051513000	47.649468000
C	41.339002000	26.451004000	54.389998000
H	41.533026000	25.885741000	55.305669000
H	40.330286000	26.214348000	54.038670000
C	42.637668000	29.961499000	55.106191000
H	41.701881000	30.426512000	54.798771000
H	42.892418000	30.286858000	56.123082000
H	43.437408000	30.287645000	54.443393000
C	43.814000000	26.436999000	51.432997000
H	44.477368000	25.659158000	51.831124000
H	43.274760000	25.994235000	50.586606000
C	46.133661000	29.475761000	51.183400000
H	46.681816000	29.179467000	50.287009000
H	45.455895000	30.304038000	50.941697000
H	46.842178000	29.808027000	51.947770000
O	40.959497000	34.223483000	52.535266000
H	41.602778000	33.497620000	52.798026000
H	41.492686000	34.832624000	52.001520000
H	40.886850000	30.714340000	45.479916000
O	38.641115000	32.014338000	49.738487000
H	38.448391000	31.148040000	50.218929000
H	39.029863000	31.808674000	48.862078000

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C	42.526834000	28.443807000	55.166180000
O	43.419090000	27.751466000	55.658550000
N	41.402681000	27.888793000	54.614162000
H	40.721668000	28.485840000	54.143143000
C	42.363106000	25.934204000	53.338878000
O	42.607933000	24.731743000	53.264045000
N	42.939253000	26.862455000	52.518068000
H	42.620459000	27.832661000	52.511171000
C	44.687916000	27.546696000	50.817333000
O	44.792788000	27.654757000	49.593513000
N	45.421990000	28.303686000	51.683195000

H	45.043317000	28.374656000	52.621110000
C	49.403051000	32.436523000	48.545630000
H	50.004977000	32.262747000	47.641798000
H	49.618204000	31.595095000	49.219029000
C	47.914225000	32.413535000	48.167380000
H	47.313176000	32.551029000	49.078294000
H	47.689814000	33.279931000	47.527421000
C	47.486653000	31.131465000	47.432042000
H	48.099935000	31.025712000	46.525414000
H	47.697514000	30.248933000	48.052463000
C	46.006597000	31.117850000	47.012692000
H	45.780760000	32.048371000	46.474350000
H	45.821987000	30.295907000	46.313266000
N	45.032509000	30.984085000	48.117718000
H	45.404889000	31.396488000	48.972800000
H	43.723466000	31.917053000	48.029689000
H	44.854915000	30.004492000	48.356417000
C	32.937254000	31.162556000	50.565079000
H	32.133697000	31.187748000	51.316870000
H	33.391704000	30.168371000	50.649385000
C	33.992336000	32.206628000	50.998292000
O	33.925837000	33.354830000	50.471925000
O	34.842556000	31.849705000	51.868284000
C	37.441173000	37.081594000	56.117773000
H	38.357090000	37.615568000	56.402760000
H	36.924137000	36.844767000	57.058710000
C	37.830834000	35.768316000	55.409378000
H	38.158421000	36.000843000	54.386790000
H	38.704616000	35.335662000	55.915202000
C	36.699096000	34.721713000	55.366029000
H	36.609445000	34.233612000	56.347312000
H	35.736187000	35.218610000	55.190424000
C	36.836711000	33.676479000	54.260483000
H	36.013305000	32.958004000	54.258116000
H	36.823722000	34.147484000	53.276526000
N	38.105287000	32.884689000	54.307970000
H	38.195517000	32.309394000	55.147736000
H	38.154339000	32.234245000	53.425516000
H	38.960039000	33.452777000	54.180547000
C	37.014294000	36.208258000	50.466484000
H	35.932576000	36.228683000	50.299204000
H	37.501756000	36.580108000	49.557356000
C	37.484083000	34.777440000	50.676092000
O	38.725301000	34.565850000	50.805313000

N	36.575537000	33.826524000	50.766263000
H	36.877287000	32.875360000	50.976051000
H	35.534607000	33.915642000	50.666561000
C	40.465155000	34.017737000	46.312757000
H	40.045793000	34.363264000	45.357096000
H	41.461461000	34.468849000	46.385743000
C	40.668908000	32.528333000	46.176982000
O	41.522118000	32.219074000	45.174506000
O	40.131195000	31.652920000	46.829558000
Mg	39.762959000	32.783596000	50.950777000
O	38.359045000	31.683438000	52.062341000
P	38.815154000	30.186684000	52.076216000
O	38.593167000	29.448173000	50.793067000
O	39.279117000	29.641128000	53.384076000
O	40.787710000	31.062428000	51.351339000
P	42.258900000	31.053734000	51.870026000
O	42.492131000	32.195529000	52.872201000
O	42.887265000	29.717915000	52.108936000
O	43.117777000	31.633103000	50.447399000
P	42.790335000	32.973982000	49.683991000
O	41.458438000	33.595809000	50.027514000
O	42.991034000	32.658219000	48.153110000
O	44.012595000	33.987737000	49.987961000
O	36.341983000	29.637907000	52.492861000
H	36.467306000	29.155627000	51.660430000
H	35.759238000	30.404514000	52.246639000
C	44.146697000	34.540452000	51.312568000
H	43.957419000	33.780797000	52.077529000
H	45.170991000	34.913785000	51.385971000
H	43.447224000	35.375042000	51.435046000
C	49.850241000	33.747972000	49.207004000
H	49.291031000	33.937187000	50.131427000
H	50.916082000	33.721474000	49.461456000
H	49.685944000	34.603732000	48.540535000
C	32.345668000	31.385014000	49.167308000
H	33.117641000	31.287921000	48.395055000
H	31.553160000	30.657758000	48.948094000
H	31.933743000	32.395178000	49.088589000
C	36.569706000	38.022298000	55.269595000
H	35.646711000	37.535832000	54.932550000
H	36.280187000	38.909729000	55.844439000
H	37.110437000	38.362117000	54.379950000
C	37.395932000	37.108521000	51.657053000
H	38.473053000	37.060848000	51.842814000

H	37.123310000	38.150661000	51.456446000
H	36.869554000	36.794822000	52.562954000
C	39.582529000	34.418979000	47.496450000
H	40.085895000	34.225789000	48.440456000
H	39.368404000	35.492815000	47.443127000
H	38.629701000	33.882709000	47.484437000
C	41.339001000	26.451005000	54.389999000
H	41.548854000	25.903056000	55.311437000
H	40.333090000	26.194799000	54.045534000
C	42.637667000	29.961499000	55.106191000
H	41.706638000	30.450065000	54.815600000
H	42.952699000	30.322147000	56.092176000
H	43.398897000	30.230717000	54.376959000
C	43.814000000	26.436999000	51.432997000
H	44.460972000	25.637399000	51.813270000
H	43.243024000	26.017219000	50.596366000
C	46.133661000	29.475761000	51.183400000
H	46.629027000	29.207111000	50.248873000
H	45.442877000	30.310366000	51.014048000
H	46.886702000	29.776236000	51.918670000
O	40.438988000	33.677606000	52.859802000
H	41.307747000	33.107891000	52.969777000
H	40.732371000	34.551220000	52.557196000
H	41.594854000	31.245769000	45.183588000
O	38.855561000	31.818913000	49.315376000
H	38.716143000	30.889324000	49.630028000
H	39.326336000	31.758919000	48.458065000
<u>dissociative Pr (-4203.609837 A.U.)</u>			
C	42.486551000	28.452129000	55.203862000
O	43.332092000	27.754223000	55.763447000
N	41.383763000	27.891885000	54.605554000
H	40.730119000	28.472833000	54.087355000
C	42.356693000	25.939925000	53.330791000
O	42.575548000	24.732932000	53.237525000
N	42.955469000	26.869404000	52.529142000
H	42.662182000	27.849684000	52.528921000
C	44.721956000	27.523445000	50.821813000
O	44.862189000	27.594384000	49.598965000
N	45.440220000	28.293766000	51.690714000
H	45.000482000	28.416787000	52.596108000
C	49.401361000	32.439959000	48.539909000
H	49.995871000	32.275374000	47.629328000
H	49.625505000	31.594210000	49.204867000
C	47.909288000	32.414588000	48.174691000

H	47.315525000	32.534712000	49.092554000
H	47.675634000	33.289127000	47.549005000
C	47.481258000	31.141417000	47.424773000
H	48.097590000	31.044474000	46.518824000
H	47.688459000	30.252224000	48.036805000
C	46.001889000	31.134911000	47.000134000
H	45.779640000	32.073206000	46.473532000
H	45.821799000	30.324169000	46.286160000
N	45.018597000	30.983831000	48.091121000
H	45.351201000	31.435637000	48.942648000
H	43.629411000	31.870295000	47.988324000
H	44.883902000	30.003201000	48.350482000
C	33.305494000	31.052004000	50.314509000
H	32.831705000	30.390298000	51.051751000
H	34.186966000	30.503481000	49.952542000
C	33.808396000	32.291391000	51.038047000
O	33.573803000	33.428199000	50.659111000
O	34.548351000	32.107611000	52.137129000
C	37.687081000	37.261540000	56.001626000
H	38.601508000	37.869218000	55.972049000
H	37.427406000	37.157913000	57.065191000
C	37.984913000	35.868486000	55.413908000
H	38.053117000	35.952314000	54.320541000
H	38.975684000	35.535900000	55.748811000
C	36.940891000	34.799068000	55.782119000
H	37.115954000	34.457648000	56.813383000
H	35.934894000	35.243107000	55.776432000
C	36.906163000	33.596271000	54.825385000
H	36.116514000	32.902249000	55.137679000
H	36.621254000	33.945635000	53.826245000
N	38.141547000	32.816825000	54.670376000
H	38.408605000	32.342306000	55.530551000
H	38.071942000	31.908713000	53.259357000
H	38.940292000	33.373650000	54.353440000
C	37.171732000	36.174641000	50.455192000
H	36.130241000	36.231442000	50.119110000
H	37.814423000	36.473682000	49.621103000
C	37.537271000	34.747098000	50.821672000
O	38.739409000	34.425655000	50.928063000
N	36.540961000	33.904201000	51.090937000
H	36.775747000	32.962702000	51.405106000
H	35.557615000	34.134835000	50.983315000
C	40.439691000	33.875008000	46.352554000
H	40.073334000	34.212823000	45.372449000

H	41.474606000	34.226008000	46.428409000
C	40.497741000	32.367272000	46.294818000
O	41.321150000	31.928270000	45.314702000
O	39.875077000	31.581668000	46.983954000
Mg	39.712390000	32.516275000	51.109497000
O	38.016512000	31.600267000	52.285113000
P	37.665037000	29.965131000	52.168536000
O	37.612521000	29.687008000	50.692375000
O	38.385222000	29.180292000	53.216437000
O	40.863200000	30.933704000	51.429154000
P	42.325749000	31.014302000	51.887503000
O	42.571246000	32.178001000	52.869533000
O	43.039901000	29.715177000	52.136717000
O	43.159161000	31.614556000	50.431337000
P	42.689390000	32.897655000	49.652685000
O	41.322370000	33.420984000	50.014860000
O	42.868122000	32.563688000	48.115593000
O	43.836254000	34.019600000	49.880800000
O	36.038846000	30.000601000	52.691240000
H	36.022426000	29.537857000	53.543668000
H	34.928274000	31.191757000	52.270032000
C	43.983283000	34.591422000	51.195347000
H	43.857086000	33.831160000	51.973426000
H	44.988624000	35.019067000	51.234389000
H	43.245435000	35.390268000	51.333530000
C	49.850241000	33.747972000	49.207004000
H	49.298477000	33.928563000	50.137567000
H	50.918484000	33.723498000	49.451942000
H	49.676996000	34.607995000	48.548212000
C	32.345668000	31.385014000	49.167308000
H	32.830801000	32.034023000	48.433201000
H	32.021679000	30.468440000	48.662981000
H	31.460019000	31.910543000	49.537823000
C	36.569706000	38.022298000	55.269595000
H	35.640494000	37.441679000	55.225199000
H	36.340411000	38.968014000	55.775515000
H	36.863852000	38.259159000	54.242172000
C	37.395932000	37.108520000	51.657053000
H	38.430725000	37.041121000	52.006331000
H	37.191176000	38.149651000	51.383346000
H	36.732080000	36.838425000	52.482837000
C	39.582529000	34.418979000	47.496449000
H	40.031421000	34.196228000	48.462805000
H	39.493315000	35.507846000	47.398882000

H	38.575734000	33.990257000	47.473209000
C	41.339000000	26.451005000	54.389998000
H	41.567397000	25.921050000	55.316615000
H	40.333691000	26.176819000	54.058493000
C	42.637669000	29.961500000	55.106192000
H	41.723288000	30.474274000	54.801933000
H	42.962407000	30.338373000	56.082197000
H	43.401247000	30.190086000	54.365446000
C	43.814001000	26.436999000	51.432997000
H	44.438909000	25.612854000	51.797461000
H	43.226435000	26.044559000	50.594669000
C	46.133661000	29.475761000	51.183400000
H	46.656512000	29.204502000	50.264525000
H	45.423193000	30.286758000	50.988558000
H	46.863167000	29.806776000	51.929397000
O	40.414428000	33.495711000	52.896024000
H	41.326192000	32.989938000	52.995794000
H	40.637438000	34.369930000	52.540181000
H	41.312143000	30.954763000	45.384011000
O	38.626064000	31.814827000	49.507785000
H	38.268752000	30.921620000	49.797441000
H	39.103335000	31.693202000	48.662630000

3. Two-lytic-water model for AceK

associative Re (-4203.625289 A.U.)

C	42.532260000	28.442607000	55.145809000
O	43.439963000	27.751280000	55.609227000
N	41.404428000	27.891649000	54.602002000
H	40.687478000	28.491071000	54.184790000
C	42.362810000	25.929231000	53.341968000
O	42.603160000	24.727207000	53.264836000
N	42.943962000	26.857042000	52.523197000
H	42.635576000	27.827432000	52.531405000
C	44.675277000	27.556531000	50.814690000
O	44.722851000	27.711414000	49.593754000
N	45.458607000	28.276945000	51.671616000
H	45.139271000	28.298859000	52.633592000
C	49.430973000	32.450043000	48.503521000
H	50.059945000	32.297665000	47.614602000
H	49.628827000	31.594879000	49.164974000
C	47.954032000	32.434252000	48.083992000
H	47.329457000	32.576350000	48.978106000
H	47.751027000	33.302001000	47.438833000
C	47.536998000	31.154945000	47.338377000

H	48.151917000	31.056664000	46.432369000
H	47.750157000	30.269700000	47.954534000
C	46.057401000	31.139601000	46.922012000
H	45.832616000	32.063544000	46.372259000
H	45.864372000	30.309131000	46.235733000
N	45.097839000	31.027912000	48.045005000
H	45.520351000	31.378183000	48.904954000
H	43.881867000	32.066424000	48.033828000
H	44.852165000	30.055004000	48.244314000
C	32.957203000	31.323909000	50.571273000
H	32.184712000	31.528375000	51.327685000
H	33.319259000	30.312657000	50.794102000
C	34.126825000	32.292398000	50.866659000
O	34.784494000	32.058818000	51.928688000
O	34.356658000	33.246737000	50.073140000
C	37.332905000	36.925131000	56.037015000
H	38.325710000	37.315548000	56.296657000
H	36.827190000	36.730713000	56.994062000
C	37.514756000	35.585983000	55.285352000
H	37.834808000	35.782209000	54.255124000
H	38.349752000	35.043425000	55.751036000
C	36.260129000	34.690739000	55.286639000
H	36.081186000	34.318743000	56.306770000
H	35.377344000	35.291513000	55.030441000
C	36.266962000	33.519333000	54.298214000
H	35.339771000	32.947717000	54.363313000
H	36.325695000	33.866806000	53.267365000
N	37.402130000	32.547224000	54.501972000
H	37.071886000	31.504805000	54.631574000
H	38.045662000	32.484007000	53.672078000
H	37.977008000	32.787632000	55.310919000
C	37.088966000	36.110792000	50.532633000
H	36.011714000	35.978886000	50.390418000
H	37.507291000	36.479132000	49.586865000
C	37.747048000	34.780860000	50.841121000
O	38.968528000	34.797193000	51.167648000
N	37.008670000	33.685832000	50.782032000
H	37.423785000	32.808015000	51.094046000
H	35.986365000	33.659266000	50.534846000
C	38.773618000	33.115483000	47.452799000
H	37.698906000	33.308799000	47.349597000
H	39.049215000	32.506238000	46.581550000
C	38.947073000	32.249071000	48.688394000
O	38.171450000	31.201697000	48.733185000

O	39.765059000	32.547660000	49.565197000
Mg	40.308441000	33.299135000	51.438732000
O	39.035369000	32.000681000	52.310564000
P	39.145480000	30.446366000	52.070447000
O	38.139391000	29.986696000	51.014440000
O	39.261620000	29.661397000	53.364616000
O	40.626712000	30.232488000	51.247850000
P	42.061242000	30.799152000	51.657779000
O	41.878336000	32.091041000	52.452382000
O	43.019820000	29.744130000	52.089653000
O	42.599861000	31.366859000	50.149897000
P	42.993300000	32.883697000	49.819461000
O	42.054149000	33.932209000	50.351021000
O	43.229928000	32.861842000	48.270984000
O	44.500214000	33.085716000	50.400483000
O	36.860624000	29.980127000	54.702593000
H	37.751848000	29.697377000	54.375575000
H	36.277600000	29.739854000	53.916281000
C	44.722753000	33.594577000	51.725566000
H	44.239905000	32.961611000	52.473518000
H	45.804678000	33.593758000	51.873587000
H	44.344690000	34.618992000	51.803187000
C	49.850241000	33.747972000	49.207004000
H	49.261515000	33.912740000	50.117796000
H	50.907855000	33.722425000	49.493655000
H	49.700712000	34.617937000	48.555726000
C	32.345667000	31.385012000	49.167307000
H	33.083421000	31.108203000	48.405912000
H	31.491394000	30.701673000	49.079379000
H	32.008700000	32.400608000	48.934881000
C	36.569704000	38.022301000	55.269598000
H	35.575031000	37.686082000	54.953118000
H	36.432036000	38.908826000	55.899680000
H	37.117997000	38.330129000	54.373239000
C	37.395932000	37.108521000	51.657053000
H	38.473010000	37.171498000	51.827933000
H	37.018732000	38.106650000	51.405368000
H	36.913296000	36.798340000	52.586957000
C	39.582526000	34.418975000	47.496456000
H	40.654915000	34.213632000	47.551634000
H	39.385458000	35.012226000	46.596143000
H	39.321724000	35.017349000	48.373084000
C	41.338999000	26.451006000	54.389996000
H	41.547202000	25.908406000	55.315092000

H	40.333421000	26.193809000	54.045933000
C	42.637672000	29.961498000	55.106179000
H	41.708422000	30.450117000	54.803978000
H	42.936942000	30.313713000	56.099555000
H	43.414603000	30.230781000	54.390068000
C	43.813996000	26.436997000	51.433001000
H	44.467093000	25.640050000	51.808456000
H	43.239814000	26.016799000	50.599037000
C	46.133664000	29.475766000	51.183401000
H	46.615389000	29.240569000	50.232638000
H	45.423765000	30.300245000	51.044323000
H	46.896688000	29.774363000	51.908930000
O	41.078599000	34.461350000	53.129907000
H	41.657230000	33.688494000	53.312468000
H	41.648482000	35.101411000	52.673354000
H	38.235728000	30.691677000	49.641736000
O	35.596499000	29.532836000	52.390915000
H	36.391252000	29.525869000	51.815131000
H	35.205235000	30.434308000	52.227394000
<u>associative TS (-4203.575555 A.U.)</u>			
C	42.477963000	28.449688000	55.244369000
O	43.293870000	27.768096000	55.861204000
N	41.393803000	27.891519000	54.612157000
H	40.821183000	28.479771000	54.011027000
C	42.380008000	25.924072000	53.356787000
O	42.615416000	24.720281000	53.291381000
N	42.974676000	26.853800000	52.549951000
H	42.613305000	27.810300000	52.503349000
C	44.705335000	27.531203000	50.821224000
O	44.857107000	27.599406000	49.601333000
N	45.400241000	28.322131000	51.690406000
H	45.001712000	28.402251000	52.618262000
C	49.413421000	32.483420000	48.455588000
H	50.010486000	32.379649000	47.538091000
H	49.639198000	31.597848000	49.066156000
C	47.922552000	32.480084000	48.089679000
H	47.331326000	32.570733000	49.012698000
H	47.692943000	33.379702000	47.499252000
C	47.481484000	31.240362000	47.293904000
H	48.072041000	31.185593000	46.367942000
H	47.706960000	30.325256000	47.860081000
C	45.990635000	31.252215000	46.917431000
H	45.758031000	32.204240000	46.420966000
H	45.775770000	30.459626000	46.193497000

N	45.055893000	31.086718000	48.050710000
H	45.465056000	31.458433000	48.908018000
H	43.761547000	32.107995000	48.099146000
H	44.863625000	30.101616000	48.243912000
C	32.383015000	32.673237000	50.008812000
H	31.961940000	33.508687000	49.438791000
H	31.773693000	32.529240000	50.910674000
C	33.814059000	33.039621000	50.452437000
O	34.342618000	32.329035000	51.359914000
O	34.370804000	34.014735000	49.871490000
C	37.157495000	36.798156000	55.993028000
H	38.180576000	37.042472000	56.307853000
H	36.593096000	36.615745000	56.919541000
C	37.204420000	35.493271000	55.168736000
H	37.639618000	35.696444000	54.182773000
H	37.904274000	34.805436000	55.662875000
C	35.841483000	34.793083000	55.014757000
H	35.502143000	34.456280000	56.007143000
H	35.084386000	35.508842000	54.668261000
C	35.807426000	33.610887000	54.035123000
H	34.839837000	33.104282000	54.069154000
H	35.940510000	33.928389000	53.000247000
N	36.859297000	32.585764000	54.294231000
H	36.788549000	31.551543000	53.693303000
H	37.782901000	32.876828000	53.949286000
H	36.939004000	32.367553000	55.289028000
C	37.220257000	36.153332000	50.477020000
H	36.172479000	36.068971000	50.173096000
H	37.796069000	36.514699000	49.615140000
C	37.770896000	34.794074000	50.851116000
O	38.924207000	34.744550000	51.361943000
N	36.988046000	33.748141000	50.649478000
H	37.316009000	32.830044000	50.934529000
H	35.989897000	33.848536000	50.327904000
C	39.540345000	32.896638000	47.296191000
H	38.797758000	32.595568000	46.550494000
H	40.517280000	32.542812000	46.938577000
C	39.266174000	32.153523000	48.589028000
O	38.672914000	30.997793000	48.464522000
O	39.605691000	32.639376000	49.669201000
Mg	40.197237000	33.184856000	51.587294000
O	38.857208000	31.945312000	52.457442000
P	38.583272000	30.468838000	52.067977000
O	37.885004000	30.112702000	50.753724000

O	39.149573000	29.299049000	53.099708000
O	40.304821000	30.222283000	51.217636000
P	41.734534000	30.659641000	51.640298000
O	41.689789000	31.938494000	52.496964000
O	42.698885000	29.581241000	52.033782000
O	42.361601000	31.291275000	50.151760000
P	42.849814000	32.786224000	49.931468000
O	41.966827000	33.867674000	50.497128000
O	43.109518000	32.867184000	48.378963000
O	44.364172000	32.880179000	50.530284000
O	37.042251000	30.391765000	53.098972000
H	38.381851000	29.128562000	53.676843000
H	36.262232000	30.087258000	52.536905000
C	44.594574000	33.312293000	51.880736000
H	44.040324000	32.691367000	52.587676000
H	45.668733000	33.214137000	52.053096000
H	44.301786000	34.361227000	51.994706000
C	49.850241000	33.747972000	49.207004000
H	49.294134000	33.862808000	50.145483000
H	50.917860000	33.717335000	49.453594000
H	49.671190000	34.647718000	48.605512000
C	32.345667000	31.385012000	49.167307000
H	32.798279000	30.552681000	49.717115000
H	31.316528000	31.108241000	48.906265000
H	32.906866000	31.514747000	48.234053000
C	36.569704000	38.022301000	55.269598000
H	35.543591000	37.844430000	54.926130000
H	36.545725000	38.891304000	55.937809000
H	37.171056000	38.289218000	54.394080000
C	37.395932000	37.108521000	51.657053000
H	38.434018000	37.110298000	51.997834000
H	37.115304000	38.131840000	51.379770000
H	36.755953000	36.810203000	52.492249000
C	39.582526000	34.418975000	47.496456000
H	40.328555000	34.683549000	48.248749000
H	39.838794000	34.917160000	46.554604000
H	38.608659000	34.796308000	47.825874000
C	41.338998000	26.451007000	54.389999000
H	41.532887000	25.917801000	55.322278000
H	40.340089000	26.187004000	54.030714000
C	42.637671000	29.961496000	55.106177000
H	41.694837000	30.477647000	54.907931000
H	43.093968000	30.345348000	56.022989000
H	43.294086000	30.162112000	54.257114000

C	43.813997000	26.436998000	51.433000000
H	44.449025000	25.611426000	51.775932000
H	43.214101000	26.051780000	50.599912000
C	46.133664000	29.475766000	51.183401000
H	46.620017000	29.188554000	50.249991000
H	45.463604000	30.325497000	50.999949000
H	46.894957000	29.769380000	51.913387000
O	41.053976000	34.324908000	53.276687000
H	41.594628000	33.514350000	53.408066000
H	41.621328000	34.914774000	52.752848000
H	38.483341000	30.586976000	49.397012000
O	35.130016000	29.751447000	51.364899000
H	35.902404000	29.786736000	50.764307000
H	34.731979000	30.660445000	51.304121000
<u>associative Pr (-4203.661440 A.U.)</u>			
C	42.454326000	28.455614000	55.283817000
O	43.207401000	27.781401000	55.977321000
N	41.399522000	27.894824000	54.597207000
H	40.880307000	28.481397000	53.954124000
C	42.332211000	25.907739000	53.327341000
O	42.545802000	24.699647000	53.268159000
N	42.905114000	26.830514000	52.501113000
H	42.574798000	27.792689000	52.511087000
C	45.101136000	27.265031000	51.242875000
O	46.127492000	26.715026000	50.840389000
N	45.014807000	28.600538000	51.459974000
H	44.105109000	29.041301000	51.650066000
C	48.889297000	32.788976000	48.488838000
H	49.142322000	32.757959000	47.419136000
H	49.048470000	31.768995000	48.865707000
C	47.399379000	33.147035000	48.636414000
H	47.136195000	33.167841000	49.703778000
H	47.223307000	34.165505000	48.261222000
C	46.494131000	32.159352000	47.879622000
H	46.778294000	32.157958000	46.818411000
H	46.682406000	31.137326000	48.239275000
C	44.985570000	32.428911000	47.937971000
H	44.751690000	33.439863000	47.590095000
H	44.464508000	31.723301000	47.284101000
N	44.403509000	32.286899000	49.306609000
H	45.046432000	31.820142000	49.948848000
H	44.104593000	33.209767000	49.748923000
H	43.468018000	31.719273000	49.363970000
C	31.860538000	32.162689000	50.401404000

H	31.342401000	33.077842000	50.098754000
H	31.158469000	31.539523000	50.969642000
C	33.021689000	32.548517000	51.321617000
O	33.596884000	31.579398000	51.940039000
O	33.361646000	33.751801000	51.406909000
C	36.354482000	36.626259000	55.880823000
H	37.284392000	36.285176000	56.355949000
H	35.609514000	36.702534000	56.686861000
C	35.877173000	35.574098000	54.865320000
H	35.014167000	35.985983000	54.321964000
H	36.662967000	35.395918000	54.121536000
C	35.449640000	34.238140000	55.503700000
H	36.324261000	33.691827000	55.881300000
H	34.828580000	34.458822000	56.382633000
C	34.610622000	33.339461000	54.575947000
H	33.852511000	32.793632000	55.144981000
H	34.084528000	33.931676000	53.820910000
N	35.349562000	32.293262000	53.801457000
H	34.696995000	31.980671000	52.986941000
H	36.256546000	32.558750000	53.375959000
H	35.569784000	31.448548000	54.336680000
C	36.367301000	36.070952000	51.232749000
H	35.457216000	36.120084000	51.844551000
H	36.038313000	36.235267000	50.199050000
C	36.943238000	34.671097000	51.336628000
O	38.092829000	34.521364000	51.802276000
N	36.176702000	33.664771000	50.905295000
H	36.536935000	32.722951000	51.044521000
H	35.160803000	33.790150000	50.842222000
C	39.605107000	32.882290000	47.496492000
H	39.138462000	32.463057000	46.599975000
H	40.641956000	32.520260000	47.525875000
C	38.945816000	32.281715000	48.719606000
O	38.297808000	31.164492000	48.500003000
O	39.032020000	32.831404000	49.819293000
Mg	39.361408000	32.900153000	51.864747000
O	37.726828000	31.720655000	52.413791000
P	37.490528000	30.247309000	52.005367000
O	37.050071000	30.088637000	50.549886000
O	38.790462000	29.392019000	52.387331000
O	42.106363000	31.119757000	49.773730000
P	41.955803000	30.964906000	51.288390000
O	40.521993000	31.251492000	51.826005000
O	42.535176000	29.718896000	51.936480000

O	42.889935000	32.238187000	51.941132000
P	42.587289000	33.832965000	51.749684000
O	41.106810000	34.091899000	52.046811000
O	43.189740000	34.351249000	50.468822000
O	43.496612000	34.449103000	52.955401000
O	36.355041000	29.646127000	52.982076000
H	39.591380000	29.955557000	52.149346000
H	35.603752000	29.259773000	52.432180000
C	43.257653000	34.077030000	54.308088000
H	43.274484000	32.988171000	54.429420000
H	44.061313000	34.516942000	54.905168000
H	42.299695000	34.474351000	54.668319000
C	49.850241000	33.747972000	49.207004000
H	49.651073000	33.776340000	50.285015000
H	50.891727000	33.437472000	49.067220000
H	49.750559000	34.771457000	48.825033000
C	32.345667000	31.385012000	49.167307000
H	32.841741000	30.454103000	49.458307000
H	31.505131000	31.130710000	48.510912000
H	33.057064000	31.981073000	48.583495000
C	36.569704000	38.022301000	55.269598000
H	35.653350000	38.387781000	54.789759000
H	36.855463000	38.746724000	56.041219000
H	37.360386000	38.012199000	54.513438000
C	37.395932000	37.108521000	51.657053000
H	38.257638000	37.100755000	50.983496000
H	36.958646000	38.113874000	51.646461000
H	37.776497000	36.903922000	52.658461000
C	39.582526000	34.418976000	47.496455000
H	40.073380000	34.807119000	48.392569000
H	40.106549000	34.805668000	46.615517000
H	38.555070000	34.799566000	47.474284000
C	41.338998000	26.451003000	54.389997000
H	41.579126000	25.944182000	55.325404000
H	40.324070000	26.174766000	54.089436000
C	42.637672000	29.961501000	55.106181000
H	41.688988000	30.497189000	55.242740000
H	43.360540000	30.309705000	55.846352000
H	42.988940000	30.166084000	54.090305000
C	43.813997000	26.436996000	51.433000000
H	44.120231000	25.409010000	51.627093000
H	43.290187000	26.444229000	50.463852000
C	46.133664000	29.475766000	51.183401000
H	47.058990000	29.049053000	51.582095000

H	46.290580000	29.627205000	50.102373000
H	45.949973000	30.441094000	51.667292000
O	39.712320000	33.088147000	54.055218000
H	40.066400000	32.186422000	54.145350000
H	40.478927000	33.622115000	53.748833000
H	37.880744000	30.776303000	49.350176000
O	34.489422000	29.087509000	51.178595000
H	35.223978000	29.355760000	50.584253000
H	34.016918000	29.934278000	51.365015000

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C	42.534030000	28.442193000	55.165946000
O	43.418810000	27.750774000	55.671364000
N	41.413090000	27.890470000	54.602721000
H	40.761848000	28.505488000	54.111432000
C	42.359958000	25.920868000	53.341099000
O	42.589289000	24.716857000	53.258269000
N	42.950388000	26.849901000	52.530725000
H	42.636554000	27.818075000	52.540479000
C	44.686274000	27.549839000	50.819347000
O	44.762505000	27.683399000	49.597239000
N	45.448333000	28.286517000	51.680853000
H	45.102489000	28.331643000	52.632761000
C	49.405344000	32.464578000	48.492291000
H	50.027828000	32.310766000	47.598951000
H	49.592027000	31.599684000	49.144228000
C	47.926373000	32.476568000	48.079072000
H	47.306858000	32.618712000	48.976610000
H	47.733359000	33.354606000	47.445021000
C	47.488373000	31.212305000	47.319351000
H	48.090073000	31.123449000	46.403579000
H	47.702625000	30.315424000	47.918102000
C	46.002845000	31.213567000	46.924062000
H	45.771554000	32.153347000	46.405038000
H	45.796501000	30.402966000	46.218114000
N	45.060441000	31.072901000	48.059311000
H	45.506815000	31.382455000	48.922364000
H	43.845079000	32.107347000	48.093203000
H	44.812375000	30.095840000	48.232576000
C	33.135603000	31.164698000	50.462584000
H	32.455832000	31.181234000	51.327264000
H	33.592434000	30.166966000	50.476937000
C	34.261344000	32.179815000	50.768815000
O	35.039982000	31.876723000	51.727751000

O	34.340731000	33.235795000	50.083116000
C	37.350760000	36.902481000	55.986073000
H	38.362320000	37.273551000	56.196824000
H	36.892634000	36.710189000	56.967211000
C	37.476538000	35.561983000	55.222495000
H	37.745021000	35.754400000	54.177652000
H	38.329303000	35.012023000	55.644786000
C	36.217786000	34.675322000	55.293002000
H	36.073444000	34.345096000	56.332888000
H	35.329047000	35.270358000	55.043967000
C	36.183666000	33.456037000	54.360125000
H	35.287367000	32.861838000	54.551104000
H	36.137966000	33.739562000	53.307933000
N	37.366303000	32.536105000	54.507994000
H	37.108679000	31.478601000	54.574998000
H	38.000186000	32.548792000	53.663011000
H	37.933274000	32.758487000	55.327721000
C	37.096247000	36.193800000	50.465532000
H	36.020563000	36.083238000	50.297135000
H	37.543104000	36.608016000	49.553139000
C	37.739107000	34.855407000	50.745547000
O	38.965189000	34.870782000	51.062738000
N	36.994579000	33.766902000	50.700130000
H	37.394540000	32.895792000	51.055239000
H	35.970427000	33.740751000	50.472403000
C	38.799280000	33.105152000	47.363545000
H	37.718859000	33.277931000	47.277032000
H	39.087828000	32.547043000	46.463610000
C	39.021263000	32.218123000	48.567901000
O	38.413117000	31.062646000	48.585832000
O	39.750206000	32.607830000	49.479798000
Mg	40.234062000	33.340071000	51.307992000
O	38.829208000	32.145247000	52.245412000
P	39.438602000	30.704496000	52.086359000
O	38.841527000	29.943904000	50.909450000
O	39.648773000	29.965799000	53.389674000
O	40.989150000	31.304645000	51.548755000
P	42.550261000	31.102221000	51.948058000
O	42.926841000	32.169761000	52.957576000
O	42.954671000	29.679533000	52.080810000
O	43.217932000	31.635392000	50.476842000
P	43.162493000	33.118894000	49.878241000
O	42.047910000	33.963769000	50.430648000
O	43.191769000	32.903273000	48.326904000

O	44.613885000	33.763288000	50.174864000
O	37.081285000	29.901864000	54.566115000
H	38.024232000	29.738661000	54.328186000
H	36.612036000	29.639553000	53.716101000
C	44.930859000	34.247378000	51.496349000
H	44.649920000	33.515026000	52.258145000
H	46.009367000	34.419247000	51.504276000
H	44.409545000	35.193152000	51.676840000
C	49.850235000	33.747969000	49.207002000
H	49.269289000	33.912830000	50.122759000
H	50.908759000	33.701300000	49.487574000
H	49.711918000	34.627112000	48.565622000
C	32.345669000	31.384998000	49.167324000
H	32.998423000	31.303246000	48.291143000
H	31.541421000	30.645295000	49.065272000
H	31.905412000	32.387257000	49.147443000
C	36.569710000	38.022302000	55.269591000
H	35.549443000	37.712424000	55.012683000
H	36.493014000	38.907801000	55.911150000
H	37.069970000	38.321419000	54.342752000
C	37.395919000	37.108470000	51.657067000
H	38.470391000	37.148433000	51.846186000
H	37.032326000	38.126598000	51.472148000
H	36.894087000	36.740301000	52.554897000
C	39.582522000	34.418978000	47.496449000
H	40.655354000	34.224834000	47.573151000
H	39.403845000	35.052816000	46.619541000
H	39.286346000	34.970240000	48.390459000
C	41.338989000	26.450985000	54.389966000
H	41.547028000	25.911856000	55.316830000
H	40.331879000	26.194027000	54.049478000
C	42.637660000	29.961503000	55.106163000
H	41.737552000	30.436042000	54.717498000
H	42.834553000	30.329047000	56.120824000
H	43.486778000	30.235782000	54.484557000
C	43.813994000	26.437016000	51.433000000
H	44.461465000	25.630099000	51.797171000
H	43.234316000	26.029124000	50.596464000
C	46.133659000	29.475758000	51.183399000
H	46.670083000	29.213343000	50.269195000
H	45.423918000	30.283791000	50.973381000
H	46.850764000	29.812818000	51.937807000
O	41.091858000	34.035072000	53.105126000
H	41.810396000	33.333391000	53.222650000

H	41.583743000	34.831692000	52.850104000
H	38.606509000	30.596461000	49.491441000
O	36.091602000	29.424875000	52.117418000
H	36.914491000	29.461752000	51.589619000
H	35.636517000	30.293084000	51.935883000
<u>dissociative TS (-4203.59129 A.U.)</u>			
C	42.508449000	28.444057000	55.220047000
O	43.358446000	27.762178000	55.793052000
N	41.410109000	27.887326000	54.617700000
H	40.786137000	28.485767000	54.073928000
C	42.357293000	25.933425000	53.333585000
O	42.576074000	24.727955000	53.236755000
N	42.962247000	26.866136000	52.536179000
H	42.645380000	27.835616000	52.532033000
C	44.724367000	27.520069000	50.823840000
O	44.874535000	27.585140000	49.603721000
N	45.431318000	28.301522000	51.693226000
H	45.010411000	28.406654000	52.609156000
C	49.344012000	32.540831000	48.405837000
H	49.886773000	32.484347000	47.451151000
H	49.584255000	31.614916000	48.946830000
C	47.835463000	32.586561000	48.122880000
H	47.296377000	32.626054000	49.080846000
H	47.593376000	33.526626000	47.604949000
C	47.330488000	31.408169000	47.273332000
H	47.896137000	31.385085000	46.330565000
H	47.536792000	30.455844000	47.782203000
C	45.834037000	31.491095000	46.930633000
H	45.622346000	32.478247000	46.498141000
H	45.578793000	30.750400000	46.165928000
N	44.910696000	31.288799000	48.068180000
H	45.338640000	31.606129000	48.937787000
H	43.616192000	32.273188000	48.128375000
H	44.708920000	30.299125000	48.222868000
C	33.350736000	32.033454000	48.207113000
H	33.696346000	31.286430000	47.481393000
H	32.882902000	32.859549000	47.660926000
C	34.561482000	32.560971000	48.991124000
O	35.359996000	31.710897000	49.475353000
O	34.650809000	33.815937000	49.144907000
C	37.638899000	37.183908000	55.992662000
H	38.550716000	37.788397000	56.084166000
H	37.311374000	36.976804000	57.021852000
C	37.999223000	35.852760000	55.299191000

H	38.148040000	36.028196000	54.226817000
H	38.966848000	35.504235000	55.685736000
C	36.947390000	34.744675000	55.496425000
H	37.004470000	34.354615000	56.523253000
H	35.939582000	35.167924000	55.392575000
C	37.020166000	33.596434000	54.488531000
H	36.232093000	32.860072000	54.669128000
H	36.894019000	33.962801000	53.468165000
N	38.308934000	32.837151000	54.484135000
H	38.450263000	32.283664000	55.331245000
H	38.331750000	32.182571000	53.609398000
H	39.153463000	33.419493000	54.316873000
C	37.235659000	36.132921000	50.493762000
H	36.214234000	36.123008000	50.102303000
H	37.909155000	36.413529000	49.674449000
C	37.638041000	34.755368000	50.963804000
O	38.761858000	34.635412000	51.544448000
N	36.774948000	33.776612000	50.808768000
H	37.062127000	32.824242000	51.030403000
H	35.923615000	33.867275000	50.186094000
C	39.599477000	32.918606000	47.181499000
H	38.833204000	32.639552000	46.447345000
H	40.564069000	32.613074000	46.758656000
C	39.381370000	32.101325000	48.432546000
O	39.391470000	30.798653000	48.296308000
O	39.213558000	32.665355000	49.513272000
Mg	39.979410000	33.030345000	51.356608000
O	38.536341000	31.731553000	52.173788000
P	39.027086000	30.263306000	51.992253000
O	38.835195000	29.641918000	50.629679000
O	39.526293000	29.542083000	53.201942000
O	40.927301000	31.233302000	51.432751000
P	42.413533000	31.135246000	51.921460000
O	42.695827000	32.183127000	53.012244000
O	42.985997000	29.762209000	52.052329000
O	43.241473000	31.817463000	50.548833000
P	42.914342000	33.241185000	49.927462000
O	41.680108000	33.912758000	50.472221000
O	42.924734000	33.020050000	48.368177000
O	44.239067000	34.133112000	50.174698000
O	36.847359000	29.665726000	52.676285000
H	37.057732000	28.775390000	52.998226000
H	36.367273000	29.514265000	51.801402000
C	44.538359000	34.553363000	51.521191000

H	44.334970000	33.752734000	52.239181000
H	45.598871000	34.815568000	51.532286000
H	43.941324000	35.436692000	51.771641000
C	49.850235000	33.747969000	49.207002000
H	49.354045000	33.811741000	50.183127000
H	50.929831000	33.683581000	49.385568000
H	49.653993000	34.686888000	48.674612000
C	32.345668000	31.384998000	49.167324000
H	31.979166000	32.117739000	49.896940000
H	31.476857000	30.978172000	48.633835000
H	32.822403000	30.568572000	49.719461000
C	36.569710000	38.022303000	55.269591000
H	35.637134000	37.463893000	55.123699000
H	36.325044000	38.920448000	55.848520000
H	36.921536000	38.344053000	54.284331000
C	37.395919000	37.108467000	51.657066000
H	38.418888000	37.080353000	52.039512000
H	37.169110000	38.136018000	51.347596000
H	36.710203000	36.853213000	52.471843000
C	39.582522000	34.418981000	47.496449000
H	40.351139000	34.664729000	48.231527000
H	39.769341000	34.997778000	46.584232000
H	38.610544000	34.717463000	47.899052000
C	41.338990000	26.450982000	54.389967000
H	41.549279000	25.902491000	55.310687000
H	40.331979000	26.196797000	54.046716000
C	42.637661000	29.961504000	55.106164000
H	41.721333000	30.441416000	54.762510000
H	42.921415000	30.358978000	56.087201000
H	43.428442000	30.197195000	54.397488000
C	43.813993000	26.437017000	51.433000000
H	44.435031000	25.607724000	51.791734000
H	43.221651000	26.051340000	50.594960000
C	46.133660000	29.475759000	51.183399000
H	46.651624000	29.195766000	50.264262000
H	45.432621000	30.293596000	50.979751000
H	46.866344000	29.805134000	51.926831000
O	40.714849000	33.672215000	53.292264000
H	41.584629000	33.067311000	53.290182000
H	41.015071000	34.572749000	53.092074000
H	39.237119000	30.366400000	49.205984000
O	35.995314000	29.206863000	50.215793000
H	36.950830000	29.245713000	50.014135000
H	35.643815000	30.063861000	49.855401000

dissociative Pr (-4203.645155 A.U.)

C	42.570112000	28.437816000	55.094028000
O	43.521427000	27.749464000	55.469338000
N	41.422998000	27.890156000	54.594986000
H	40.634709000	28.492874000	54.307618000
C	42.408647000	25.928776000	53.391640000
O	42.754755000	24.753631000	53.398447000
N	42.914750000	26.847911000	52.501770000
H	42.440356000	27.740218000	52.436635000
C	44.746432000	27.486357000	50.835466000
O	45.104486000	27.366094000	49.664181000
N	45.174421000	28.482936000	51.649917000
H	44.887011000	28.471818000	52.621076000
C	48.841852000	32.820690000	48.516050000
H	49.124290000	32.708301000	47.458582000
H	48.904811000	31.815726000	48.955682000
C	47.391281000	33.321816000	48.596909000
H	47.051045000	33.319879000	49.641049000
H	47.355415000	34.369024000	48.260783000
C	46.432568000	32.497069000	47.720966000
H	46.827804000	32.463950000	46.696138000
H	46.395191000	31.453924000	48.065208000
C	45.013208000	33.065256000	47.633298000
H	45.036894000	34.151863000	47.508891000
H	44.472760000	32.647153000	46.779050000
N	44.178494000	32.812249000	48.847667000
H	44.711198000	32.808228000	49.768138000
H	43.458779000	33.598788000	48.954579000
H	43.686789000	31.916589000	48.813731000
C	33.790237000	30.876434000	49.140605000
H	33.961136000	30.111236000	49.909881000
H	34.014202000	30.377211000	48.188046000
C	34.827175000	31.979187000	49.329875000
O	36.105025000	31.611294000	49.343849000
O	34.524298000	33.159186000	49.443525000
C	37.860063000	37.599804000	55.991864000
H	38.622754000	38.371086000	55.817565000
H	37.687495000	37.588732000	57.078396000
C	38.416543000	36.231140000	55.550736000
H	38.379779000	36.154635000	54.456940000
H	39.477608000	36.167160000	55.822761000
C	37.677417000	35.030061000	56.164737000
H	37.933182000	34.951948000	57.233161000
H	36.592077000	35.202173000	56.129272000

C	37.940349000	33.691392000	55.463236000
H	37.316223000	32.914907000	55.937074000
H	37.630793000	33.766488000	54.418071000
N	39.361811000	33.302162000	55.440602000
H	39.670940000	32.999387000	56.363751000
H	39.481872000	32.512904000	54.792467000
H	40.492960000	34.142978000	54.511327000
C	37.471471000	35.863453000	50.765235000
H	36.566343000	35.760419000	50.156434000
H	38.331220000	35.949505000	50.091450000
C	37.714532000	34.610697000	51.585259000
O	38.705489000	34.549221000	52.347976000
N	36.825913000	33.620652000	51.489328000
H	37.049405000	32.721302000	51.924781000
H	36.114196000	33.627723000	50.761118000
C	39.436334000	32.903101000	47.633700000
H	38.427716000	32.572851000	47.348397000
H	40.121112000	32.367616000	46.964301000
C	39.666232000	32.368052000	49.036362000
O	39.776667000	31.072793000	49.091412000
O	39.715533000	33.123750000	50.016133000
Mg	40.529363000	33.475630000	51.911420000
O	39.846754000	31.851885000	52.891226000
P	39.123139000	30.506788000	52.672973000
O	39.277230000	29.953737000	51.234712000
O	39.268406000	29.521277000	53.812538000
O	42.446673000	32.801737000	51.513540000
P	43.766198000	33.413529000	51.975653000
O	43.829713000	33.536964000	53.574646000
O	45.041414000	32.810159000	51.430977000
O	43.728305000	35.006750000	51.485235000
P	42.525029000	35.569734000	50.503799000
O	41.205519000	35.406805000	51.243373000
O	42.700892000	35.019090000	49.105678000
O	42.928854000	37.141722000	50.436770000
O	37.442960000	30.919611000	52.717276000
H	37.160017000	30.719895000	53.624362000
H	36.598920000	29.789540000	51.400251000
C	42.800874000	37.939835000	51.612254000
H	43.468120000	37.578901000	52.403828000
H	43.089074000	38.957418000	51.334148000
H	41.767127000	37.939693000	51.975233000
C	49.850235000	33.747969000	49.207002000
H	49.613733000	33.867511000	50.270904000

H	50.869688000	33.351882000	49.132453000
H	49.843698000	34.746464000	48.752504000
C	32.345668000	31.384998000	49.167324000
H	32.180695000	32.129363000	48.382893000
H	31.644813000	30.556512000	49.016795000
H	32.116888000	31.863694000	50.124349000
C	36.569710000	38.022303000	55.269591000
H	35.784384000	37.262026000	55.360587000
H	36.171986000	38.956151000	55.685726000
H	36.753617000	38.183923000	54.203763000
C	37.395919000	37.108468000	51.657066000
H	38.306224000	37.199323000	52.254610000
H	37.290657000	38.012961000	51.047400000
H	36.535626000	37.054981000	52.332338000
C	39.582522000	34.418981000	47.496449000
H	40.566123000	34.755354000	47.837117000
H	39.447550000	34.716445000	46.449498000
H	38.827090000	34.936914000	48.093686000
C	41.338991000	26.450981000	54.389966000
H	41.496658000	25.891103000	55.316250000
H	40.344830000	26.218968000	53.996424000
C	42.637660000	29.961506000	55.106165000
H	41.720356000	30.433439000	54.743730000
H	42.857329000	30.300857000	56.124116000
H	43.470511000	30.288180000	54.474575000
C	43.813991000	26.437015000	51.433000000
H	44.421193000	25.616736000	51.832681000
H	43.264022000	26.022128000	50.578627000
C	46.133660000	29.475760000	51.183399000
H	47.125466000	29.305576000	51.623491000
H	46.209773000	29.359776000	50.101183000
H	45.798882000	30.488218000	51.432247000
O	41.200535000	34.368538000	53.810898000
H	42.933733000	33.818391000	53.888277000
H	41.056658000	35.279307000	53.501602000
H	39.676205000	30.684420000	50.084805000
O	36.698011000	29.382698000	50.512002000
H	37.690473000	29.359954000	50.504925000
H	36.285128000	30.649203000	49.640948000

4. Double Mg²⁺ model for AceK

associative Re (-4556.515315 A.U.)

C	42.522701000	28.443875000	55.209963000
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O	43.384577000	27.765562000	55.753946000
N	41.423278000	27.885795000	54.603907000
H	40.719770000	28.493039000	54.193373000
C	42.258618000	25.892297000	53.268024000
O	42.315832000	24.684287000	53.076233000
N	42.958674000	26.818451000	52.547450000
H	42.722587000	27.796111000	52.668307000
C	45.111751000	27.259028000	51.270150000
O	46.213329000	26.734611000	51.295694000
N	44.963978000	28.615026000	51.001801000
H	44.086287000	29.029603000	51.314707000
C	49.405773000	32.436968000	48.546707000
H	49.941249000	32.305998000	47.596652000
H	49.694130000	31.587504000	49.180434000
C	47.894207000	32.378042000	48.276467000
H	47.366241000	32.501373000	49.236122000
H	47.602445000	33.236774000	47.654662000
C	47.455415000	31.079596000	47.577936000
H	48.030331000	30.957875000	46.651431000
H	47.695433000	30.206078000	48.199117000
C	45.979187000	31.046124000	47.180067000
H	45.703727000	31.941067000	46.615322000
H	45.738117000	30.170534000	46.573082000
N	45.052646000	31.011192000	48.370634000
H	45.388785000	31.618091000	49.126796000
H	44.096379000	31.421037000	48.151467000
H	44.947342000	30.071892000	48.780090000
C	32.649429000	31.321793000	50.670462000
H	32.754166000	32.320776000	51.104665000
H	31.825187000	30.817226000	51.189718000
C	33.913772000	30.529751000	50.913905000
O	34.913503000	31.048716000	51.517764000
O	33.987182000	29.338666000	50.467969000
C	37.597177000	37.316697000	56.167141000
H	38.498575000	37.937970000	56.231542000
H	37.210883000	37.239261000	57.192134000
C	37.986641000	35.911126000	55.668202000
H	38.139979000	35.957640000	54.579441000
H	38.955135000	35.626294000	56.099353000
C	36.939881000	34.826766000	56.006894000
H	37.129263000	34.427843000	57.011261000
H	35.937465000	35.271057000	56.042071000
C	36.862195000	33.686320000	54.991896000
H	36.169761000	32.904473000	55.315780000

H	36.516165000	34.057817000	54.023762000
N	38.181943000	33.023929000	54.744956000
H	38.506161000	32.391885000	55.526221000
H	38.164955000	32.431609000	53.879051000
H	38.926705000	33.709107000	54.556913000
C	36.627384000	36.011017000	50.905849000
H	35.569834000	35.997522000	51.192254000
H	36.661265000	36.206632000	49.825706000
C	37.254153000	34.653202000	51.141433000
O	38.504704000	34.561136000	51.176153000
N	36.465289000	33.593647000	51.335776000
H	36.880429000	32.677694000	51.520460000
H	35.457853000	33.632057000	51.271133000
C	38.890152000	33.062903000	47.229550000
H	37.802036000	33.178308000	47.285396000
H	39.153975000	32.674409000	46.243477000
C	39.309255000	32.084365000	48.284709000
O	40.081620000	31.098960000	47.864806000
O	38.985588000	32.193743000	49.477223000
Mg	39.807220000	33.022971000	51.372545000
O	38.464308000	31.711670000	52.262878000
P	38.810389000	30.189342000	52.471137000
O	37.733256000	29.270309000	51.891353000
O	39.248378000	29.852314000	53.876922000
O	40.101632000	29.909074000	51.419256000
P	41.549667000	30.608401000	51.638214000
O	41.303925000	31.917574000	52.383456000
O	42.599869000	29.656300000	52.079490000
O	41.869231000	31.075732000	50.067635000
P	42.431906000	32.608190000	49.696258000
O	41.405398000	33.614329000	50.193631000
O	42.808247000	32.508842000	48.244827000
O	43.829152000	32.710472000	50.531158000
O	39.360725000	31.136001000	56.238525000
H	39.379224000	30.524317000	55.459024000
H	39.219401000	30.586782000	57.023058000
C	44.000990000	33.526183000	51.706719000
H	43.598629000	33.009964000	52.580162000
H	45.076113000	33.673587000	51.822913000
H	43.511140000	34.493792000	51.572663000
C	49.850245000	33.747972000	49.207006000
H	49.361265000	33.892538000	50.178209000
H	50.931578000	33.752533000	49.377018000
H	49.607593000	34.612658000	48.577890000

C	32.345670000	31.385019000	49.167293000
H	32.229747000	30.377562000	48.760359000
H	31.422112000	31.942654000	48.981543000
H	33.155414000	31.881599000	48.620333000
C	36.569708000	38.022328000	55.269590000
H	35.688063000	37.396877000	55.080050000
H	36.214420000	38.946830000	55.736886000
H	37.007195000	38.292425000	54.304165000
C	37.395943000	37.108497000	51.657044000
H	38.431811000	37.154405000	51.313630000
H	36.928487000	38.082542000	51.484677000
H	37.395789000	36.918409000	52.731528000
C	39.582551000	34.418942000	47.496451000
H	40.669244000	34.313031000	47.460737000
H	39.275523000	35.134783000	46.727778000
H	39.307035000	34.812727000	48.477154000
C	41.339009000	26.451011000	54.389993000
H	41.622968000	25.919435000	55.301909000
H	40.308453000	26.181358000	54.142540000
C	42.637667000	29.961492000	55.106186000
H	41.698342000	30.456559000	54.856117000
H	43.012139000	30.343684000	56.060586000
H	43.371454000	30.193229000	54.331591000
C	43.814003000	26.436992000	51.433005000
H	44.111707000	25.399676000	51.585986000
H	43.260376000	26.488468000	50.480182000
C	46.133662000	29.475747000	51.183405000
H	46.856713000	29.337487000	50.371358000
H	45.795853000	30.516442000	51.211201000
H	46.663338000	29.254657000	52.117725000
O	40.407462000	34.150531000	53.235095000
H	41.120991000	33.487455000	53.362924000
H	40.832470000	35.001486000	53.042742000
H	40.508443000	30.676837000	48.648241000
Mg	35.979684000	29.286497000	51.013616000
O	35.589510000	27.925362000	52.630575000
H	34.816188000	27.990130000	53.211335000
H	36.387218000	28.073731000	53.170943000
O	36.122819000	27.560204000	49.743898000
H	36.379892000	26.749150000	50.212943000
H	35.198668000	27.427491000	49.467024000
O	36.812547000	30.235398000	49.291910000
H	37.272090000	29.523319000	48.815916000
H	37.510533000	30.864602000	49.563537000

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C	42.483486000	28.450788000	55.279039000
O	43.271682000	27.787783000	55.938847000
N	41.423085000	27.883837000	54.608182000
H	40.846855000	28.494234000	54.044858000
C	42.231942000	25.892530000	53.245412000
O	42.236399000	24.690205000	53.011117000
N	42.980892000	26.812550000	52.568138000
H	42.742470000	27.791558000	52.681968000
C	45.095914000	27.273405000	51.252641000
O	46.198362000	26.749173000	51.202114000
N	44.941522000	28.636821000	51.057658000
H	44.066254000	29.055700000	51.376420000
C	49.413969000	32.438872000	48.536000000
H	49.946410000	32.323617000	47.582129000
H	49.715680000	31.586309000	49.159345000
C	47.901617000	32.361533000	48.270096000
H	47.372494000	32.456712000	49.232025000
H	47.594675000	33.226504000	47.664353000
C	47.485003000	31.068443000	47.547088000
H	48.068010000	30.972602000	46.622546000
H	47.737079000	30.188496000	48.154651000
C	46.011721000	31.012875000	47.138173000
H	45.719101000	31.916682000	46.596312000
H	45.798765000	30.150901000	46.501613000
N	45.075506000	30.917641000	48.314239000
H	45.357228000	31.539703000	49.079919000
H	44.089792000	31.266521000	48.091531000
H	45.021074000	29.973735000	48.719739000
C	32.552693000	31.483335000	50.686311000
H	32.626832000	32.524466000	51.014115000
H	31.701648000	31.023479000	51.202410000
C	33.807998000	30.739140000	51.076196000
O	34.816413000	31.354423000	51.562109000
O	33.870674000	29.483178000	50.857816000
C	36.665488000	37.352301000	56.648330000
H	37.368231000	37.926841000	57.264681000
H	35.694239000	37.423501000	57.156668000
C	37.122225000	35.877477000	56.672067000
H	38.090715000	35.795752000	56.152222000
H	37.329242000	35.614578000	57.715681000
C	36.112395000	34.845648000	56.103880000
H	36.093746000	33.946748000	56.734094000
H	35.098374000	35.261104000	56.153861000

C	36.35776000	34.41098200	54.65648600
H	35.50883300	33.84705200	54.26011200
H	36.51453600	35.28002800	54.01443600
N	37.55533400	33.51535300	54.52584000
H	37.33760500	32.40066600	54.54917000
H	38.00483700	33.58461200	53.60606900
H	38.27671200	33.75314300	55.21038000
C	36.71338800	36.09574200	50.72832800
H	35.62901000	36.07522100	50.88153700
H	36.89101000	36.37408400	49.68221600
C	37.31804700	34.73252000	50.96177900
O	38.56797600	34.63279500	50.99959400
N	36.51782800	33.69103500	51.19121600
H	36.93525800	32.79086200	51.43032400
H	35.51022300	33.72810400	51.13028500
C	38.82163200	33.10341000	47.20911800
H	37.74089100	33.27687500	47.25963900
H	39.07093500	32.71499400	46.21916500
C	39.17928600	32.08761700	48.25341900
O	39.90906100	31.07258300	47.82544000
O	38.85180600	32.19495500	49.44442100
Mg	39.86778100	33.09880600	51.30287700
O	38.48488300	31.96462300	52.26854600
P	38.58001200	30.49904800	52.76791100
O	37.60051400	29.42767200	52.27182200
O	39.52447200	30.11720200	54.03787700
O	39.89192000	29.97858300	51.67195500
P	41.37446000	30.57730300	51.69787100
O	41.31853400	31.95885200	52.35757800
O	42.42501000	29.59032300	52.07975700
O	41.63295900	30.95734100	50.06975000
P	42.35194800	32.38877400	49.62132600
O	41.42159200	33.51983900	50.04283000
O	42.73409800	32.19761600	48.17811400
O	43.75891100	32.44081400	50.45080600
O	37.33268600	30.98138700	54.28268800
H	38.93527500	30.19656500	54.81593500
H	36.46177800	30.58318800	54.12546600
C	43.99401200	33.31538000	51.57304300
H	43.57596100	32.87422400	52.47832300
H	45.07784500	33.41180200	51.66424800
H	43.55329000	34.29777200	51.38668900
C	49.85024500	33.74797200	49.20700600
H	49.36556200	33.87882000	50.18227900

H	50.932493000	33.760120000	49.370729000
H	49.596261000	34.616436000	48.587632000
C	32.345670000	31.385019000	49.167294000
H	32.257179000	30.339243000	48.862434000
H	31.435034000	31.912786000	48.866480000
H	33.188439000	31.828388000	48.624886000
C	36.569708000	38.022328000	55.269590000
H	35.823906000	37.538916000	54.626338000
H	36.274452000	39.071743000	55.372031000
H	37.535511000	37.999992000	54.750470000
C	37.395943000	37.108497000	51.657044000
H	38.467602000	37.149649000	51.451451000
H	36.975609000	38.107898000	51.508239000
H	37.257447000	36.844835000	52.708565000
C	39.582551000	34.418941000	47.496451000
H	40.662160000	34.256505000	47.469134000
H	39.319844000	35.156495000	46.731504000
H	39.321287000	34.817675000	48.478285000
C	41.339007000	26.451018000	54.389993000
H	41.651817000	25.933750000	55.300209000
H	40.304604000	26.166564000	54.175598000
C	42.637666000	29.961490000	55.106187000
H	41.716662000	30.466389000	54.816791000
H	43.017625000	30.372404000	56.046135000
H	43.382361000	30.140730000	54.326856000
C	43.814009000	26.436987000	51.433002000
H	44.125861000	25.402354000	51.573885000
H	43.240020000	26.486521000	50.492270000
C	46.133658000	29.475747000	51.183406000
H	46.831008000	29.289828000	50.359061000
H	45.819555000	30.523616000	51.183443000
H	46.681951000	29.273154000	52.111313000
O	40.383596000	34.218155000	53.147339000
H	41.022623000	33.497083000	53.342440000
H	40.906918000	35.018877000	52.984456000
H	40.321773000	30.633983000	48.608744000
Mg	35.856276000	29.512074000	51.367080000
O	35.114898000	28.755307000	53.263313000
H	34.201771000	28.426122000	53.247624000
H	35.644922000	28.152141000	53.807039000
O	36.541554000	27.641035000	50.563793000
H	37.355223000	27.469355000	51.071397000
H	36.079056000	26.798984000	50.434618000
O	36.711824000	30.240153000	49.558355000

H	37.146418000	29.473873000	49.148876000
H	37.419893000	30.905681000	49.689199000
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C	42.260164000	28.505283000	55.418771000
O	42.723054000	27.923268000	56.386988000
N	41.397073000	27.909748000	54.519614000
H	41.215666000	28.446147000	53.675269000
C	42.274678000	25.874119000	53.293704000
O	42.362138000	24.663912000	53.142369000
N	42.961865000	26.799685000	52.555528000
H	42.664740000	27.764513000	52.599449000
C	45.120635000	27.238676000	51.352524000
O	46.207210000	26.683551000	51.271009000
N	44.979090000	28.604573000	51.329668000
H	44.046897000	29.004525000	51.318149000
C	48.802142000	34.760778000	48.732737000
H	49.118831000	35.774478000	49.014113000
H	48.751511000	34.750785000	47.635163000
C	47.396652000	34.506213000	49.301565000
H	47.077381000	33.492755000	49.010892000
H	47.439184000	34.513744000	50.400307000
C	46.375947000	35.552514000	48.825264000
H	46.734116000	36.553305000	49.098321000
H	46.316283000	35.548317000	47.726730000
C	44.969953000	35.419866000	49.408717000
H	44.974321000	35.398157000	50.501532000
H	44.325942000	36.243395000	49.089681000
N	44.267543000	34.158401000	48.984620000
H	44.732879000	33.333500000	49.371587000
H	43.233886000	34.137814000	49.367396000
H	44.253736000	34.061948000	47.965457000
C	32.601111000	31.138309000	50.659257000
H	32.553628000	32.067051000	51.237733000
H	31.808852000	30.491243000	51.062464000
C	33.917563000	30.446647000	50.983616000
O	34.552180000	30.776727000	52.039905000
O	34.362678000	29.517132000	50.234255000
C	36.905775000	37.916031000	56.763384000
H	37.782484000	38.541229000	56.972420000
H	36.083313000	38.343504000	57.352584000
C	37.206072000	36.500192000	57.289937000
H	38.093747000	36.103198000	56.771678000
H	37.501535000	36.587364000	58.341710000
C	36.034524000	35.496942000	57.203547000

H	36.089654000	34.776204000	58.031244000
H	35.085584000	36.029532000	57.343310000
C	35.926713000	34.714174000	55.893551000
H	34.990038000	34.153846000	55.835084000
H	36.001362000	35.361519000	55.020317000
N	37.023080000	33.697381000	55.748914000
H	36.968096000	32.978760000	56.479563000
H	36.981926000	33.160619000	54.843367000
H	37.968270000	34.102643000	55.762113000
C	36.210433000	36.161959000	51.838630000
H	35.544955000	36.538773000	52.628745000
H	35.597695000	36.117253000	50.929796000
C	36.626032000	34.753176000	52.231877000
O	37.729689000	34.552702000	52.793522000
N	35.744864000	33.772628000	52.006014000
H	35.931925000	32.809381000	52.285487000
H	34.875932000	33.954639000	51.524597000
C	38.450338000	34.085253000	48.475316000
H	38.208459000	34.938216000	49.114154000
H	37.542174000	33.811799000	47.920772000
C	38.807508000	32.924624000	49.368179000
O	39.251585000	31.880440000	48.712404000
O	38.673982000	32.962802000	50.598331000
Mg	38.997441000	32.884044000	52.653890000
O	37.325139000	31.959182000	53.643443000
P	37.355389000	30.587759000	54.345193000
O	36.833821000	29.397445000	53.569446000
O	38.828039000	30.328595000	54.930292000
O	39.698864000	29.977140000	50.424208000
P	40.699687000	30.432624000	51.526392000
O	39.915708000	31.059213000	52.724113000
O	41.756879000	29.442202000	51.931688000
O	41.488497000	31.739313000	50.817688000
P	41.814823000	33.266227000	51.251963000
O	40.894965000	33.698712000	52.391626000
O	41.871300000	34.112764000	49.996515000
O	43.367193000	33.217944000	51.742055000
O	36.493990000	30.815499000	55.709121000
H	39.449834000	30.341648000	54.139357000
H	36.168479000	29.973632000	56.071260000
C	43.763627000	32.412664000	52.864617000
H	43.522738000	31.361993000	52.686342000
H	44.843104000	32.534903000	52.972311000
H	43.271793000	32.758514000	53.779103000

C	49.850245000	33.747972000	49.207006000
H	49.584761000	32.726935000	48.907750000
H	50.832207000	33.974071000	48.779496000
H	49.951331000	33.760660000	50.298676000
C	32.345670000	31.385019000	49.167293000
H	32.401820000	30.447897000	48.607123000
H	31.353930000	31.822154000	49.015294000
H	33.086199000	32.072775000	48.742314000
C	36.569708000	38.022328000	55.269590000
H	35.604462000	37.559494000	55.029415000
H	36.501556000	39.071878000	54.964945000
H	37.343854000	37.549476000	54.654071000
C	37.395943000	37.108497000	51.657044000
H	38.031378000	36.790560000	50.824242000
H	37.040601000	38.121675000	51.447089000
H	38.021296000	37.135600000	52.551263000
C	39.582551000	34.418941000	47.496451000
H	39.781484000	33.573709000	46.832779000
H	39.304192000	35.281303000	46.881839000
H	40.496355000	34.655590000	48.046589000
C	41.339009000	26.451012000	54.389994000
H	41.640773000	26.019070000	55.345728000
H	40.317814000	26.119411000	54.174255000
C	42.637666000	29.961491000	55.106186000
H	41.944330000	30.452336000	54.421083000
H	42.710840000	30.509989000	56.049080000
H	43.631221000	29.952328000	54.644621000
C	43.814004000	26.436993000	51.433005000
H	44.081179000	25.386151000	51.540656000
H	43.272137000	26.555138000	50.481017000
C	46.133662000	29.475746000	51.183405000
H	46.133613000	29.990922000	50.212344000
H	46.169629000	30.226533000	51.982622000
H	47.022048000	28.845706000	51.244258000
O	39.703157000	33.265558000	54.746501000
H	39.864109000	32.358229000	55.069075000
H	40.553951000	33.576604000	54.372289000
H	39.538445000	31.130806000	49.342150000
Mg	36.024673000	29.303391000	51.722132000
O	34.995672000	27.459040000	51.827778000
H	34.359077000	27.647640000	51.109431000
H	35.515634000	26.689788000	51.541989000
O	37.783290000	27.990801000	51.352686000
H	38.548673000	28.444467000	50.926155000

H	38.099673000	27.762404000	52.242924000
O	37.053071000	30.502512000	50.397741000
H	36.752566000	30.385637000	49.482867000
H	38.043045000	30.388547000	50.412306000
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C	42.637875000	28.452297000	54.967122000
O	43.653764000	27.782016000	55.133995000
N	41.439942000	27.883812000	54.626440000
H	40.643898000	28.486636000	54.450693000
C	42.288951000	25.918909000	53.277982000
O	42.553298000	24.724888000	53.223394000
N	42.765735000	26.826213000	52.373053000
H	42.589447000	27.819404000	52.494478000
C	44.571654000	27.639359000	50.826760000
O	44.456227000	27.952875000	49.629731000
N	45.438570000	28.279640000	51.644582000
H	45.335431000	28.135776000	52.643499000
C	49.453975000	32.342578000	48.717328000
H	50.079394000	32.077582000	47.853710000
H	49.690685000	31.606027000	49.497746000
C	47.973387000	32.186395000	48.312593000
H	47.333647000	32.399433000	49.183231000
H	47.719837000	32.943717000	47.557110000
C	47.667104000	30.786363000	47.738876000
H	48.349793000	30.598694000	46.900261000
H	47.893182000	30.008795000	48.481021000
C	46.251963000	30.578960000	47.181063000
H	45.969658000	31.412406000	46.531830000
H	46.190617000	29.657297000	46.597972000
N	45.176498000	30.487277000	48.236092000
H	45.358598000	31.136128000	49.012232000
H	44.254503000	30.836547000	47.884369000
H	45.040309000	29.537704000	48.656551000
C	32.845971000	30.305471000	50.140756000
H	32.385381000	30.458092000	51.126343000
H	32.569053000	29.302600000	49.804440000
C	34.350545000	30.366723000	50.332188000
O	34.891392000	31.489256000	50.556104000
O	35.025148000	29.277316000	50.243796000
C	37.604403000	37.229188000	56.086994000
H	38.469433000	37.877538000	56.273425000
H	37.189423000	36.992393000	57.076270000
C	38.106290000	35.923251000	55.429460000
H	38.330005000	36.111439000	54.369973000

H	39.062113000	35.644641000	55.896784000
C	37.122644000	34.743560000	55.549748000
H	37.042849000	34.437390000	56.602977000
H	36.114623000	35.069041000	55.262790000
C	37.427481000	33.523619000	54.678780000
H	36.689361000	32.727961000	54.797211000
H	37.446428000	33.780024000	53.618660000
N	38.781849000	32.910826000	54.955954000
H	38.950508000	32.817135000	55.961426000
H	38.893115000	31.936396000	54.523243000
H	39.527938000	33.492752000	54.542058000
C	37.079453000	36.170073000	50.478121000
H	35.998400000	36.102305000	50.316971000
H	37.533838000	36.558370000	49.560434000
C	37.673197000	34.808020000	50.746289000
O	38.922119000	34.692811000	50.810225000
N	36.853869000	33.777318000	50.973016000
H	37.256153000	32.887615000	51.285522000
H	35.848993000	33.843498000	50.880400000
C	40.010093000	33.065936000	46.934278000
H	39.527427000	32.835736000	45.978139000
H	41.093068000	33.033632000	46.757031000
C	39.716709000	31.943923000	47.881649000
O	39.686613000	30.746813000	47.328861000
O	39.489239000	32.099877000	49.093765000
Mg	40.179101000	33.125252000	51.068571000
O	38.757513000	31.911279000	51.825423000
P	38.983085000	30.487823000	52.395371000
O	37.889283000	29.500272000	51.938840000
O	39.297906000	30.455027000	53.877347000
O	40.334170000	29.889907000	51.520933000
P	41.824547000	30.609633000	51.625352000
O	41.575149000	31.974867000	52.263067000
O	42.847465000	29.671176000	52.148364000
O	42.114120000	30.933997000	50.036941000
P	42.712837000	32.369692000	49.456848000
O	41.831006000	33.510435000	49.950841000
O	42.945875000	32.116067000	47.997275000
O	44.188967000	32.477902000	50.162433000
O	35.747041000	31.085849000	53.380015000
H	36.318510000	30.320380000	53.199067000
H	35.415820000	31.330064000	52.495865000
C	44.454536000	33.371209000	51.261586000
H	43.974223000	33.003516000	52.171058000

H	45.538232000	33.381706000	51.392228000
H	44.101073000	34.377539000	51.025733000
C	49.850241000	33.747972000	49.207004000
H	49.278343000	34.039277000	50.096511000
H	50.912596000	33.778456000	49.468515000
H	49.672797000	34.503535000	48.432785000
C	32.345669000	31.385013000	49.167310000
H	32.769731000	31.243517000	48.166984000
H	31.255740000	31.343840000	49.078480000
H	32.628702000	32.379866000	49.520754000
C	36.569702000	38.022302000	55.269599000
H	35.684231000	37.421973000	55.026858000
H	36.224754000	38.895279000	55.833176000
H	37.001242000	38.384084000	54.330065000
C	37.395931000	37.108522000	51.657055000
H	38.475752000	37.177996000	51.813348000
H	37.011830000	38.112826000	51.454257000
H	36.926925000	36.750008000	52.577151000
C	39.582528000	34.418975000	47.496452000
H	40.142788000	34.665169000	48.398405000
H	39.769405000	35.201436000	46.753701000
H	38.512805000	34.431312000	47.731008000
C	41.338999000	26.451004000	54.389996000
H	41.597098000	25.881297000	55.286824000
H	40.306420000	26.213621000	54.118616000
C	42.637669000	29.961500000	55.106183000
H	41.692191000	30.422930000	54.812568000
H	42.853548000	30.212054000	56.152198000
H	43.441796000	30.362942000	54.489670000
C	43.814000000	26.437008000	51.433004000
H	44.521040000	25.771693000	51.943384000
H	43.399321000	25.880303000	50.585938000
C	46.133657000	29.475758000	51.183401000
H	46.680245000	29.247441000	50.265686000
H	45.430648000	30.300517000	51.024027000
H	46.857108000	29.771821000	51.946811000
O	40.690043000	34.176825000	53.091955000
H	41.384823000	33.478089000	53.138409000
H	41.135734000	35.036894000	53.035719000
H	39.502782000	30.064666000	48.022720000
Mg	37.049139000	29.198277000	50.214718000
O	36.573992000	27.159858000	50.101631000
H	36.835067000	26.555481000	50.815721000
H	35.601020000	27.252132000	50.153614000

O	39.048538000	28.820375000	49.344235000
H	39.668046000	29.087386000	50.077046000
H	39.302371000	27.919900000	49.079617000
O	37.051835000	30.919685000	49.158828000
H	37.851979000	31.469283000	49.301536000
H	36.278655000	31.378044000	49.594981000

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C	42.619405000	28.447742000	55.010078000
O	43.618135000	27.773419000	55.242704000
N	41.427465000	27.879125000	54.646721000
H	40.670390000	28.478782000	54.345505000
C	42.303749000	25.918204000	53.291097000
O	42.568766000	24.722446000	53.244421000
N	42.791902000	26.825189000	52.398685000
H	42.558601000	27.818018000	52.463426000
C	44.538080000	27.662426000	50.828257000
O	44.375601000	28.017844000	49.650069000
N	45.429456000	28.283220000	51.637349000
H	45.375188000	28.096943000	52.632431000
C	49.348628000	32.404188000	48.646511000
H	49.871802000	32.194450000	47.703299000
H	49.631855000	31.595193000	49.334206000
C	47.829336000	32.333732000	48.387163000
H	47.291767000	32.484721000	49.336340000
H	47.532757000	33.166609000	47.733774000
C	47.408972000	31.004882000	47.724023000
H	48.007353000	30.868385000	46.814025000
H	47.661240000	30.154267000	48.371601000
C	45.942911000	30.904759000	47.279924000
H	45.639552000	31.811460000	46.748846000
H	45.793493000	30.053644000	46.611551000
N	44.957061000	30.732905000	48.408119000
H	45.214716000	31.294119000	49.228212000
H	44.017670000	31.141609000	48.167196000
H	44.835346000	29.750483000	48.743409000
C	33.144243000	30.080722000	49.199944000
H	32.503213000	29.241779000	49.502683000
H	33.501375000	29.816332000	48.195811000
C	34.363470000	30.049597000	50.120718000
O	34.670059000	31.051027000	50.808107000
O	35.012960000	28.934667000	50.128089000
C	37.606899000	37.252314000	56.102119000
H	38.494145000	37.884608000	56.227897000
H	37.215449000	37.078976000	57.113897000

C	38.045808000	35.901933000	55.497331000
H	38.257898000	36.030068000	54.426855000
H	38.994813000	35.598985000	55.961945000
C	37.005679000	34.783436000	55.689204000
H	36.936785000	34.522108000	56.755233000
H	36.009321000	35.149160000	55.410724000
C	37.231953000	33.518598000	54.863189000
H	36.460749000	32.769269000	55.049998000
H	37.227751000	33.729009000	53.791876000
N	38.557160000	32.852303000	55.133420000
H	38.721317000	32.731992000	56.136639000
H	38.592766000	31.888930000	54.674211000
H	39.336420000	33.402584000	54.720914000
C	36.935791000	36.111356000	50.581668000
H	35.851816000	36.168117000	50.434144000
H	37.406493000	36.362301000	49.622466000
C	37.353944000	34.693348000	50.912681000
O	38.545133000	34.464163000	51.234041000
N	36.436495000	33.724198000	50.868471000
H	36.711616000	32.764504000	51.079645000
H	35.479248000	33.890236000	50.591895000
C	39.690037000	32.982716000	46.983586000
H	38.848772000	32.713609000	46.329328000
H	40.604604000	32.820350000	46.405883000
C	39.722150000	32.034288000	48.140938000
O	40.181795000	30.803802000	47.893468000
O	39.347963000	32.356785000	49.266749000
Mg	39.784348000	32.851524000	51.283997000
O	38.137026000	31.502511000	51.603373000
P	38.075401000	30.297941000	52.554573000
O	37.476403000	28.992020000	52.071253000
O	38.605338000	30.405899000	53.953685000
O	40.060872000	29.496745000	51.456015000
P	41.352659000	30.321308000	51.699380000
O	40.949778000	31.624770000	52.441121000
O	42.581048000	29.614335000	52.184447000
O	41.741805000	30.934587000	50.146201000
P	42.455290000	32.403237000	49.866209000
O	41.578316000	33.488008000	50.485076000
O	42.765598000	32.389313000	48.393740000
O	43.899031000	32.351602000	50.632878000
O	36.023786000	30.936081000	53.115776000
H	35.678091000	30.168436000	53.601829000
H	35.509053000	30.940925000	52.244951000

C	44.078923000	32.792151000	51.991609000
H	43.704934000	32.035266000	52.683737000
H	45.153519000	32.928841000	52.130564000
H	43.569124000	33.746176000	52.146794000
C	49.850241000	33.747972000	49.207004000
H	49.380218000	33.981022000	50.170114000
H	50.933459000	33.720059000	49.361606000
H	49.629776000	34.572605000	48.519113000
C	32.345669000	31.385013000	49.167310000
H	32.964618000	32.218617000	48.819297000
H	31.490871000	31.290646000	48.490159000
H	31.969045000	31.643987000	50.161765000
C	36.569702000	38.022302000	55.269599000
H	35.677004000	37.421301000	55.056634000
H	36.235336000	38.917418000	55.804424000
H	36.993972000	38.349293000	54.315006000
C	37.395931000	37.108522000	51.657055000
H	38.477341000	37.045591000	51.801348000
H	37.143648000	38.129696000	51.356378000
H	36.901272000	36.906246000	52.610124000
C	39.582528000	34.418975000	47.496452000
H	40.407256000	34.647066000	48.175422000
H	39.618627000	35.119668000	46.656060000
H	38.641802000	34.576592000	48.030507000
C	41.339006000	26.451006000	54.389989000
H	41.583710000	25.878349000	55.288279000
H	40.310395000	26.212714000	54.104044000
C	42.637668000	29.961499000	55.106183000
H	41.699612000	30.432507000	54.804640000
H	42.872068000	30.239425000	56.140810000
H	43.436470000	30.330763000	54.463040000
C	43.813993000	26.437007000	51.433011000
H	44.537365000	25.774423000	51.922556000
H	43.384181000	25.885617000	50.589183000
C	46.133658000	29.475759000	51.183401000
H	46.607625000	29.270695000	50.220961000
H	45.449166000	30.327028000	51.103501000
H	46.915148000	29.716978000	51.908073000
O	40.476544000	33.887474000	53.377890000
H	41.061173000	33.091085000	53.265618000
H	40.999603000	34.671236000	53.147690000
H	40.601614000	30.482988000	48.735905000
Mg	36.958511000	28.489947000	50.251672000
O	36.099530000	26.593770000	50.030494000

H	36.166501000	25.854415000	50.654465000
H	35.170495000	26.903623000	50.032701000
O	38.892334000	27.827963000	49.824878000
H	39.490105000	28.346889000	50.457878000
H	39.218798000	26.916652000	49.798534000
O	37.521560000	30.129263000	49.133417000
H	38.328990000	29.960347000	48.614675000
H	37.782202000	30.820330000	49.786014000
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C	42.480200000	28.440743000	55.238670000
O	43.309130000	27.770619000	55.841953000
N	41.383287000	27.893085000	54.622910000
H	40.903971000	28.442561000	53.912133000
C	42.471029000	25.940541000	53.447865000
O	43.018786000	24.862990000	53.628961000
N	42.801818000	26.794260000	52.420694000
H	42.111513000	27.500473000	52.152615000
C	44.453601000	27.727319000	50.874761000
O	44.048613000	28.291993000	49.849968000
N	45.498886000	28.230082000	51.580933000
H	45.730585000	27.819496000	52.475435000
C	49.028040000	32.608850000	48.567344000
H	49.281218000	32.551764000	47.499484000
H	49.343550000	31.649733000	49.001259000
C	47.490926000	32.729514000	48.691612000
H	47.204458000	32.705055000	49.754244000
H	47.170450000	33.709182000	48.309356000
C	46.761660000	31.620106000	47.898164000
H	47.143149000	31.637928000	46.868959000
H	47.030933000	30.629158000	48.288289000
C	45.231821000	31.728386000	47.765936000
H	44.928528000	32.760540000	47.567850000
H	44.876594000	31.111857000	46.936821000
N	44.431587000	31.286665000	48.965237000
H	44.771621000	31.717963000	49.830076000
H	43.416252000	31.625235000	48.914961000
H	44.415119000	30.258395000	49.122278000
C	32.800721000	29.934200000	49.374949000
H	31.935167000	29.256100000	49.387084000
H	33.441097000	29.585844000	48.558086000
C	33.558223000	29.687265000	50.656868000
O	33.342912000	30.591601000	51.581807000
O	34.299159000	28.702912000	50.817630000
C	37.901715000	37.434815000	55.754502000

H	38.717530000	37.856424000	55.154032000
H	38.091345000	37.754310000	56.788248000
C	37.978776000	35.900137000	55.667592000
H	37.724890000	35.588382000	54.644594000
H	39.019651000	35.586770000	55.827278000
C	37.064155000	35.172160000	56.669569000
H	37.508840000	35.191108000	57.674364000
H	36.106368000	35.698522000	56.757572000
C	36.720241000	33.740259000	56.271287000
H	36.054691000	33.267983000	56.999365000
H	36.221403000	33.715612000	55.298009000
N	37.908427000	32.838606000	56.135952000
H	38.381285000	32.687432000	57.029856000
H	37.573266000	31.891890000	55.714423000
H	38.603856000	33.171443000	55.444360000
C	36.165807000	36.210559000	51.618340000
H	35.370736000	36.593329000	52.271269000
H	35.740489000	36.194580000	50.604784000
C	36.462526000	34.771924000	52.001022000
O	37.640097000	34.353903000	52.066147000
N	35.410922000	33.987089000	52.270095000
H	35.586258000	32.986720000	52.427668000
H	34.467913000	34.329592000	52.153627000
C	38.286477000	33.599096000	47.660718000
H	37.470432000	34.230974000	48.021467000
H	37.999110000	33.164278000	46.697877000
C	38.498721000	32.479886000	48.647029000
O	39.133539000	31.455030000	48.152043000
O	38.118456000	32.557311000	49.829941000
Mg	38.541349000	32.498992000	51.845067000
O	36.697082000	31.572149000	52.483130000
P	36.408545000	30.513089000	53.589227000
O	36.465514000	29.064480000	53.070829000
O	37.037162000	30.721156000	54.949718000
O	39.390056000	29.671729000	49.993148000
P	40.120548000	29.784692000	51.378418000
O	39.294645000	30.684006000	52.328197000
O	40.515315000	28.446472000	51.944098000
O	41.529474000	30.649470000	51.123490000
P	41.689506000	32.229826000	50.740804000
O	40.569142000	33.040129000	51.396549000
O	41.971433000	32.358387000	49.266362000
O	43.115670000	32.573448000	51.476268000
O	34.744339000	30.799754000	53.803999000

H	34.451175000	30.373994000	54.627034000
H	33.872348000	30.466403000	52.428819000
C	43.154914000	33.095103000	52.808020000
H	42.701143000	32.400730000	53.523037000
H	44.208450000	33.224512000	53.065825000
H	42.651646000	34.066057000	52.855826000
C	49.850241000	33.747972000	49.207004000
H	49.667190000	33.820351000	50.285778000
H	50.920450000	33.572818000	49.059676000
H	49.602345000	34.717206000	48.758917000
C	32.345669000	31.385013000	49.167310000
H	33.200951000	32.067828000	49.154173000
H	31.826555000	31.473971000	48.208314000
H	31.663215000	31.705523000	49.958140000
C	36.569702000	38.022302000	55.269599000
H	35.723404000	37.697293000	55.886012000
H	36.592187000	39.116481000	55.309759000
H	36.358777000	37.734437000	54.234586000
C	37.395931000	37.108522000	51.657055000
H	38.153175000	36.760720000	50.949601000
H	37.123131000	38.134956000	51.393009000
H	37.856442000	37.121226000	52.647766000
C	39.582528000	34.418975000	47.496452000
H	40.407946000	33.778042000	47.177580000
H	39.431844000	35.204957000	46.749793000
H	39.870517000	34.888049000	48.442289000
C	41.339000000	26.451003000	54.389996000
H	41.459629000	25.909087000	55.328524000
H	40.364800000	26.209057000	53.955247000
C	42.637669000	29.961501000	55.106183000
H	41.674180000	30.483740000	55.078458000
H	43.234561000	30.324576000	55.944847000
H	43.170752000	30.177173000	54.172449000
C	43.814000000	26.437008000	51.433003000
H	44.549754000	25.793560000	51.922201000
H	43.392153000	25.891949000	50.579143000
C	46.133657000	29.475758000	51.183401000
H	46.383040000	29.437421000	50.120603000
H	45.485066000	30.338909000	51.384141000
H	47.057475000	29.599667000	51.753234000
O	39.576709000	32.740721000	53.902553000
H	39.678184000	31.769699000	53.723725000
H	40.303580000	33.138875000	53.380373000
H	39.339834000	30.754342000	48.868955000

Mg	36.284842000	28.346717000	51.261039000
O	35.895309000	26.549303000	52.290458000
H	35.919122000	26.910018000	53.197456000
H	35.084065000	26.024198000	52.209778000
O	37.927095000	27.468675000	50.408118000
H	38.582293000	28.160490000	50.091010000
H	38.458935000	26.888605000	50.978903000
O	36.716286000	30.031445000	50.197104000
H	37.701391000	30.026165000	50.043298000
H	36.601762000	30.755239000	50.860574000

5. Model for AceK-ICDH

associative Re (-4395.604049 A.U.)

C	71.448027000	60.735227000	31.209982000
O	72.310617000	59.948794000	30.813078000
N	71.712143000	61.671437000	32.168336000
H	70.971617000	62.256643000	32.564592000
C	73.422103000	60.541471000	33.667163000
O	74.602975000	60.340885000	33.941274000
N	72.394662000	59.784425000	34.138768000
H	71.434121000	60.036133000	33.916828000
C	71.771759000	57.402486000	34.717942000
O	71.586908000	56.574444000	35.607004000
N	71.294651000	57.266731000	33.446839000
H	71.371084000	58.086283000	32.857795000
C	65.242026000	53.170431000	32.079509000
H	65.884949000	54.001374000	32.395285000
H	64.696363000	53.524539000	31.192536000
C	64.231074000	52.834070000	33.186550000
H	63.609063000	51.990683000	32.855330000
H	64.770825000	52.480873000	34.077549000
C	63.312461000	54.003926000	33.579795000
H	62.807847000	54.386595000	32.679092000
H	62.518732000	53.640013000	34.248453000
C	64.060253000	55.153824000	34.262044000
H	64.508959000	54.811886000	35.201979000
H	64.880755000	55.512201000	33.636524000
N	63.236427000	56.341268000	34.578507000
H	62.516101000	56.117615000	35.264386000
H	64.310334000	57.481904000	35.009179000
H	62.753420000	56.667426000	33.741170000
C	66.103640000	68.005169000	38.845935000
H	66.010973000	69.068964000	39.105179000

H	67.057042000	67.682130000	39.282923000
C	66.253812000	67.919505000	37.320049000
O	67.261981000	68.543122000	36.843020000
O	65.398935000	67.278777000	36.658329000
C	63.893814000	66.311364000	31.317435000
H	64.189708000	65.340289000	31.733413000
H	64.344259000	66.365213000	30.316447000
C	64.448294000	67.433346000	32.205516000
H	64.230849000	68.410787000	31.748704000
H	63.892709000	67.419704000	33.154069000
C	65.950886000	67.332953000	32.533686000
H	66.201351000	66.293955000	32.777444000
H	66.560186000	67.614282000	31.663643000
C	66.258562000	68.216577000	33.742878000
H	66.122708000	69.277911000	33.504708000
H	65.575723000	67.970625000	34.561162000
N	67.621217000	68.070796000	34.340070000
H	68.307863000	68.693800000	33.914209000
H	67.512889000	68.305799000	35.452575000
H	68.054847000	67.118297000	34.291600000
C	62.938367000	64.864429000	34.987135000
H	62.895101000	65.947521000	34.820396000
H	62.849309000	64.730400000	36.073336000
C	64.295361000	64.344714000	34.555947000
O	64.332814000	63.354910000	33.778638000
N	65.379093000	64.957774000	35.010405000
H	66.279738000	64.554731000	34.723119000
H	65.340736000	65.741063000	35.673953000
C	64.815720000	61.213514000	37.891167000
H	64.498492000	61.962770000	38.625612000
H	65.551119000	60.578492000	38.403110000
C	65.620200000	61.927825000	36.821557000
O	65.591135000	61.584538000	35.635640000
O	66.336655000	62.917764000	37.297429000
C	69.463719000	60.847370000	39.768894000
H	69.852566000	61.694008000	40.343764000
H	70.297251000	60.143099000	39.640006000
C	69.042136000	61.327876000	38.390029000
O	68.175818000	60.762901000	37.745464000
O	69.708853000	62.411388000	37.999431000
O	67.242452000	63.339045000	33.757643000
P	68.575820000	63.038748000	34.488176000
O	68.494502000	63.575447000	35.942020000
O	69.829978000	63.396262000	33.717063000

O	68.590251000	61.359115000	34.752869000
P	68.279736000	60.230478000	33.665392000
O	67.387269000	60.822908000	32.580043000
O	69.472020000	59.405841000	33.335916000
O	67.187308000	59.224775000	34.516877000
P	65.729081000	58.852925000	34.009987000
O	64.920610000	59.996859000	33.438588000
O	65.108750000	58.094278000	35.236385000
O	65.861322000	57.653023000	32.923900000
Mg	65.801902000	61.981718000	33.522141000
O	69.448184000	66.036196000	34.632714000
H	69.227904000	65.537556000	35.444226000
H	69.745860000	65.292706000	34.057708000
C	66.413189000	57.878776000	31.615328000
H	67.488168000	58.061814000	31.681214000
H	66.225616000	56.965354000	31.046352000
H	65.926008000	58.726661000	31.126547000
C	66.126789000	51.982015000	31.695881000
H	66.832688000	52.251541000	30.902548000
H	66.712111000	51.631657000	32.554583000
H	65.526248000	51.136594000	31.336553000
C	70.163179000	56.391444000	33.159156000
H	70.204630000	56.071772000	32.112291000
H	70.236008000	55.516131000	33.807616000
H	69.214827000	56.906106000	33.348659000
C	72.623034000	58.656971000	35.017016000
H	72.411518000	58.904601000	36.064270000
H	73.685840000	58.403601000	34.950535000
C	73.032994000	61.737024000	32.780001000
H	73.070597000	62.641239000	33.395461000
H	73.808836000	61.805189000	32.012842000
C	70.034184000	60.698192000	30.637991000
H	70.105334000	60.838720000	29.552906000
H	69.612839000	59.711883000	30.832137000
H	69.369615000	61.452547000	31.061682000
C	68.291755000	60.164557000	40.471254000
H	67.910740000	59.345078000	39.856875000
H	68.592865000	59.763551000	41.446611000
H	67.469139000	60.870108000	40.634501000
C	64.938028000	67.198099000	39.416220000
H	65.049541000	66.135008000	39.180001000
H	64.881859000	67.304607000	40.506850000
H	63.986701000	67.527820000	38.986237000
C	62.363476000	66.367999000	31.201856000

H	61.978378000	65.535417000	30.601823000
H	61.888739000	66.316906000	32.187927000
H	62.033297000	67.301422000	30.726731000
C	61.830353000	64.128503000	34.247834000
H	61.847718000	63.061149000	34.483437000
H	60.847861000	64.526846000	34.530363000
H	61.942219000	64.222323000	33.165891000
C	63.637433000	60.372281000	37.385575000
H	63.136197000	59.888230000	38.232015000
H	62.899737000	60.993731000	36.864379000
H	63.982500000	59.602520000	36.693736000
H	69.329668000	62.755996000	37.132280000
H	67.097321000	63.196504000	36.670843000
O	65.270852000	61.845386000	31.387159000
H	66.181791000	61.525881000	31.223565000
H	64.777856000	61.020026000	31.549351000
<u>associative TS (-4395.560534 A.U.)</u>			
C	71.481562000	60.835635000	31.106349000
O	72.389216000	60.221618000	30.550410000
N	71.714495000	61.670144000	32.166723000
H	70.940419000	62.099174000	32.663510000
C	73.441177000	60.527772000	33.644075000
O	74.629389000	60.303851000	33.860427000
N	72.413661000	59.800830000	34.155243000
H	71.456890000	60.108444000	34.000007000
C	71.928654000	57.340696000	34.598865000
O	72.064959000	56.338753000	35.297898000
N	71.180358000	57.383093000	33.460467000
H	70.986300000	58.304275000	33.093919000
C	65.305239000	53.194437000	32.141532000
H	65.990785000	53.995644000	32.444326000
H	64.733987000	53.585753000	31.286962000
C	64.333379000	52.870910000	33.286559000
H	63.675602000	52.048704000	32.971811000
H	64.900451000	52.491820000	34.149476000
C	63.461723000	54.057392000	33.733096000
H	62.924990000	54.461320000	32.860804000
H	62.691355000	53.702119000	34.433186000
C	64.260398000	55.184451000	34.395788000
H	64.758641000	54.817075000	35.300583000
H	65.047046000	55.552310000	33.732842000
N	63.463604000	56.368819000	34.786851000
H	62.771999000	56.126090000	35.495756000
H	64.540105000	57.503637000	35.217094000

H	62.944864000	56.722741000	33.982619000
C	66.053498000	68.089864000	38.870761000
H	65.840714000	69.146041000	39.093466000
H	67.013280000	67.871658000	39.353013000
C	66.255021000	67.979656000	37.348003000
O	67.351993000	68.427442000	36.900564000
O	65.309980000	67.485293000	36.665913000
C	63.870828000	66.120664000	31.367630000
H	64.036426000	65.124973000	31.799016000
H	64.354499000	66.108335000	30.380743000
C	64.531319000	67.176360000	32.262795000
H	64.434530000	68.167370000	31.792775000
H	63.958226000	67.237924000	33.199381000
C	66.006434000	66.919674000	32.623731000
H	66.135422000	65.887918000	32.971093000
H	66.646803000	67.038778000	31.738058000
C	66.409919000	67.882617000	33.740068000
H	66.385227000	68.920898000	33.385168000
H	65.705156000	67.804492000	34.573355000
N	67.746434000	67.649349000	34.364705000
H	68.495187000	68.125210000	33.860669000
H	67.676047000	68.038700000	35.369414000
H	68.109043000	66.598141000	34.505235000
C	62.813617000	64.838737000	35.174465000
H	62.799808000	65.926419000	35.035142000
H	62.551443000	64.670253000	36.227677000
C	64.221799000	64.323098000	34.945208000
O	64.354320000	63.308212000	34.211537000
N	65.238666000	64.951610000	35.515056000
H	66.177507000	64.607836000	35.287317000
H	65.145657000	65.836885000	36.037948000
C	65.019671000	60.580371000	38.004428000
H	64.963448000	60.977980000	39.022483000
H	65.548559000	59.619403000	38.069037000
C	65.908752000	61.487724000	37.178267000
O	65.779280000	61.570412000	35.955264000
O	66.807570000	62.127913000	37.879218000
C	69.787551000	60.315693000	40.131206000
H	70.263039000	60.989677000	40.853006000
H	70.290455000	59.345288000	40.171973000
C	69.970400000	60.878394000	38.729648000
O	70.217364000	60.203851000	37.750861000
O	69.776237000	62.206746000	38.715728000
O	67.287244000	63.457464000	34.284777000

P	68.606171000	63.219362000	35.033534000
O	68.662183000	63.381321000	36.554972000
O	69.975876000	63.362811000	34.171590000
O	68.691897000	61.469771000	35.029420000
P	68.387294000	60.440939000	33.870256000
O	67.454041000	61.070266000	32.837642000
O	69.570593000	59.659368000	33.418793000
O	67.349755000	59.330997000	34.674040000
P	65.887949000	58.935732000	34.203156000
O	65.037772000	60.078094000	33.693675000
O	65.326600000	58.136832000	35.434006000
O	66.013294000	57.770770000	33.081161000
Mg	65.889626000	62.074513000	33.873636000
O	68.950003000	65.417725000	34.883513000
H	69.204458000	65.596469000	35.803114000
H	70.028365000	64.367096000	34.170822000
C	66.502507000	58.070568000	31.761148000
H	67.557019000	58.352954000	31.799795000
H	66.383870000	57.154365000	31.179012000
H	65.920618000	58.877225000	31.306278000
C	66.126789000	51.982015000	31.695881000
H	66.806934000	52.241499000	30.877162000
H	66.735352000	51.592121000	32.520695000
H	65.478903000	51.167607000	31.347633000
C	70.163182000	56.391445000	33.159158000
H	70.185316000	56.125836000	32.094996000
H	70.372856000	55.499957000	33.754504000
H	69.164098000	56.769069000	33.413372000
C	72.623029000	58.656979000	35.017007000
H	72.260573000	58.867690000	36.031586000
H	73.699117000	58.478449000	35.075373000
C	73.032987000	61.737014000	32.780004000
H	73.070468000	62.632096000	33.409664000
H	73.795924000	61.825330000	32.003975000
C	70.034191000	60.698193000	30.637994000
H	70.017158000	60.830753000	29.550757000
H	69.696535000	59.686050000	30.867535000
H	69.346185000	61.401403000	31.110024000
C	68.291755000	60.164557000	40.471255000
H	67.810950000	59.463488000	39.780230000
H	68.163874000	59.780769000	41.490354000
H	67.778527000	61.126562000	40.388953000
C	64.938027000	67.198099000	39.416221000
H	65.164690000	66.139425000	39.246779000

H	64.801133000	67.345238000	40.495443000
H	63.993075000	67.414011000	38.909342000
C	62.363476000	66.367999000	31.201856000
H	61.895357000	65.593619000	30.582554000
H	61.853655000	66.373268000	32.172042000
H	62.170388000	67.337651000	30.724358000
C	61.830354000	64.128503000	34.247834000
H	61.809156000	63.055378000	34.452956000
H	60.817538000	64.526754000	34.386493000
H	62.108755000	64.254528000	33.199774000
C	63.637433000	60.372281000	37.385575000
H	63.059652000	59.653300000	37.978157000
H	63.073462000	61.311601000	37.353451000
H	63.727347000	59.996720000	36.365619000
H	69.657218000	62.531373000	37.783537000
H	67.479877000	62.643140000	37.294836000
O	65.306591000	62.089294000	31.733420000
H	66.194894000	61.723087000	31.544124000
H	64.754009000	61.294053000	31.834316000

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C	71.494270000	61.055341000	30.960002000
O	72.403938000	60.816573000	30.170017000
N	71.698404000	61.644130000	32.184270000
H	70.894752000	61.644317000	32.811249000
C	73.443265000	60.523006000	33.639026000
O	74.626017000	60.210366000	33.749275000
N	72.418911000	59.876052000	34.263049000
H	71.469829000	60.239579000	34.198144000
C	71.975853000	57.389968000	34.434056000
O	72.458806000	56.281340000	34.662630000
N	70.843043000	57.554001000	33.703266000
H	70.394754000	58.464946000	33.640640000
C	65.510882000	53.377451000	31.833331000
H	66.176389000	54.002691000	32.441686000
H	65.461495000	53.856619000	30.844980000
C	64.104229000	53.347806000	32.448708000
H	63.469465000	52.681069000	31.847993000
H	64.155547000	52.894375000	33.450082000
C	63.418513000	54.720758000	32.549531000
H	63.370992000	55.182672000	31.552099000
H	62.376719000	54.579465000	32.874127000
C	64.106021000	55.690224000	33.518952000
H	64.176769000	55.236062000	34.515185000
H	65.130638000	55.901848000	33.198339000

N	63.438285000	56.995185000	33.672596000
H	62.480977000	56.882682000	34.003370000
H	64.467429000	58.022549000	34.446345000
H	63.402424000	57.485974000	32.778966000
C	66.349804000	67.557027000	38.946961000
H	66.736015000	68.422841000	39.503436000
H	67.046753000	66.734841000	39.146873000
C	66.443674000	67.896396000	37.454011000
O	67.636643000	67.932317000	36.961214000
O	65.404183000	68.104848000	36.793529000
C	63.890374000	66.250807000	31.148201000
H	64.198023000	65.225003000	31.381404000
H	64.242154000	66.439510000	30.124817000
C	64.573918000	67.224281000	32.121330000
H	64.584974000	68.239901000	31.698175000
H	63.966009000	67.294837000	33.034552000
C	65.989602000	66.800129000	32.538864000
H	65.954485000	65.756101000	32.871804000
H	66.673906000	66.824217000	31.680201000
C	66.499741000	67.690949000	33.669856000
H	66.836238000	68.667900000	33.307101000
H	65.727290000	67.872603000	34.422676000
N	67.632860000	67.092638000	34.443043000
H	68.533994000	67.149735000	33.964983000
H	67.694257000	67.581609000	35.407849000
H	67.484523000	66.083121000	34.671300000
C	62.665529000	65.187574000	34.962393000
H	62.633963000	66.136369000	34.410460000
H	62.250998000	65.405808000	35.953918000
C	64.128311000	64.801942000	35.141575000
O	64.651959000	63.882499000	34.468633000
N	64.817870000	65.489611000	36.048377000
H	65.805506000	65.244872000	36.154619000
H	64.510602000	66.369032000	36.458855000
C	64.955420000	60.565319000	38.138478000
H	64.848591000	60.430443000	39.220089000
H	65.688064000	59.820919000	37.795502000
C	65.605867000	61.901844000	37.873352000
O	65.395138000	62.547313000	36.844176000
O	66.423226000	62.312742000	38.814854000
C	69.738761000	60.692531000	40.401568000
H	70.064551000	61.030669000	41.391298000
H	70.419096000	59.914660000	40.045439000
C	69.781266000	61.849801000	39.432051000

O	70.116999000	61.718586000	38.261056000
O	69.338379000	62.980158000	39.974934000
O	67.429450000	64.467250000	35.610001000
P	68.562391000	64.502713000	36.674400000
O	68.046397000	64.247755000	38.099394000
O	69.752597000	63.534636000	36.273213000
O	67.722721000	61.230117000	35.611003000
P	68.218223000	61.038717000	34.166945000
O	67.682878000	62.253482000	33.361765000
O	69.606213000	60.520816000	33.877083000
O	67.214878000	59.708506000	33.585809000
P	65.647948000	59.771785000	33.778905000
O	65.127730000	61.136573000	34.152003000
O	65.230938000	58.618242000	34.778173000
O	65.025149000	59.219609000	32.383278000
Mg	66.364884000	62.709046000	34.998770000
O	69.286491000	65.934582000	36.595648000
H	68.725548000	66.668496000	36.983398000
H	69.871501000	62.790686000	36.924042000
C	65.433725000	59.844161000	31.143538000
H	66.478214000	59.594860000	30.934905000
H	64.789544000	59.423953000	30.367258000
H	65.313416000	60.931299000	31.187559000
C	66.126789000	51.982015000	31.695881000
H	67.126725000	52.029984000	31.250806000
H	66.221939000	51.493061000	32.673227000
H	65.508023000	51.335235000	31.060883000
C	70.163173000	56.391441000	33.159155000
H	70.808086000	55.860786000	32.449611000
H	69.887250000	55.684584000	33.951295000
H	69.259310000	56.727531000	32.645038000
C	72.623041000	58.656978000	35.017011000
H	72.249237000	58.777546000	36.043729000
H	73.696712000	58.472997000	35.070619000
C	73.032987000	61.737020000	32.780006000
H	73.093024000	62.642072000	33.396267000
H	73.761524000	61.812987000	31.972775000
C	70.034190000	60.698192000	30.637992000
H	69.921522000	60.669037000	29.551852000
H	69.817837000	59.704915000	31.046191000
H	69.319672000	61.397167000	31.081298000
C	68.291755000	60.164557000	40.471254000
H	67.962200000	59.823027000	39.485683000
H	68.230254000	59.319484000	41.167056000

H	67.607878000	60.947966000	40.804672000
C	64.938028000	67.198099000	39.416220000
H	64.587852000	66.276513000	38.938542000
H	64.916989000	67.037556000	40.500717000
H	64.229202000	67.993410000	39.166314000
C	62.363476000	66.367999000	31.201856000
H	61.884723000	65.688755000	30.486411000
H	61.979490000	66.122562000	32.197371000
H	62.030269000	67.387120000	30.963301000
C	61.830353000	64.128503000	34.247834000
H	61.818325000	63.192514000	34.814911000
H	60.797824000	64.474703000	34.127817000
H	62.239075000	63.904468000	33.259483000
C	63.637433000	60.372281000	37.385575000
H	63.249764000	59.362787000	37.561202000
H	62.880412000	61.090965000	37.721541000
H	63.792350000	60.506535000	36.313968000
H	69.048802000	63.612870000	39.247580000
H	66.951587000	63.121271000	38.491373000
O	65.579898000	63.138558000	31.713248000
H	66.430921000	62.830336000	32.098082000
H	64.972049000	63.036369000	32.464512000

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C	71.483737000	60.810672000	31.113383000
O	72.385226000	60.168574000	30.574177000
N	71.715845000	61.653907000	32.164713000
H	70.935704000	62.100374000	32.650559000
C	73.438561000	60.536138000	33.654717000
O	74.623354000	60.329839000	33.906155000
N	72.410981000	59.784752000	34.134160000
H	71.455016000	60.083319000	33.962353000
C	71.891379000	57.347990000	34.638116000
O	71.921033000	56.395812000	35.414685000
N	71.240011000	57.330320000	33.439221000
H	71.152467000	58.223280000	32.974828000
C	65.181292000	53.022099000	32.300177000
H	65.690667000	53.993557000	32.318241000
H	64.303953000	53.146957000	31.648559000
C	64.706324000	52.647274000	33.712073000
H	64.207258000	51.669171000	33.671390000
H	65.579703000	52.515416000	34.367165000
C	63.746631000	53.668588000	34.345914000
H	62.895286000	53.838174000	33.668575000

H	63.326683000	53.252188000	35.273189000
C	64.416778000	55.009640000	34.658024000
H	65.228665000	54.871411000	35.381119000
H	64.865058000	55.444175000	33.761642000
N	63.514351000	56.045920000	35.207988000
H	63.102567000	55.740577000	36.089666000
H	64.388547000	57.348860000	35.328576000
H	62.742705000	56.217627000	34.563690000
C	64.996163000	68.394657000	38.451215000
H	63.995640000	68.601573000	38.053760000
H	65.346966000	69.281361000	38.990991000
C	65.954185000	68.119664000	37.276540000
O	67.166020000	68.411571000	37.464461000
O	65.456318000	67.595094000	36.233325000
C	63.806037000	65.851230000	31.262316000
H	63.814519000	64.850671000	31.713743000
H	64.198127000	65.727504000	30.242949000
C	64.749575000	66.756301000	32.069287000
H	64.868410000	67.723293000	31.558521000
H	64.289240000	66.984364000	33.040569000
C	66.120445000	66.107929000	32.318455000
H	65.967030000	65.098576000	32.714479000
H	66.659910000	65.984159000	31.368250000
C	66.967751000	66.901000000	33.313538000
H	67.355508000	67.829122000	32.880200000
H	66.402317000	67.165694000	34.215099000
N	68.143801000	66.106960000	33.799375000
H	68.847714000	65.950259000	33.074263000
H	68.587078000	66.620912000	34.629028000
H	67.846289000	65.144360000	34.119853000
C	62.766791000	64.998025000	35.079238000
H	62.795664000	66.033879000	34.717994000
H	62.437833000	65.055329000	36.124135000
C	64.164603000	64.417211000	35.041856000
O	64.348265000	63.415760000	34.302109000
N	65.115606000	64.960031000	35.787005000
H	66.048907000	64.550649000	35.701515000
H	65.048685000	65.930163000	36.148693000
C	65.050083000	60.271008000	37.957671000
H	65.092278000	60.579128000	39.010490000
H	65.418898000	59.239704000	37.924148000
C	66.035308000	61.113781000	37.178742000
O	65.649778000	61.826644000	36.244386000
O	67.274572000	61.017275000	37.560861000

C	69.823690000	60.180885000	40.298036000
H	70.261545000	60.930948000	40.967577000
H	70.249443000	59.203593000	40.541915000
C	70.211326000	60.507401000	38.865334000
O	70.583993000	59.686777000	38.053466000
O	70.045061000	61.816789000	38.604078000
O	67.369242000	63.600765000	34.633757000
P	68.636137000	62.674538000	34.743127000
O	68.996802000	62.347162000	36.190400000
O	69.712425000	62.995149000	33.750587000
O	67.746424000	61.248593000	34.228333000
P	68.068601000	59.939900000	33.307353000
O	67.359149000	60.130218000	31.980946000
O	69.473852000	59.492243000	33.443907000
O	67.084750000	58.829533000	34.153111000
P	65.492383000	58.881675000	34.103008000
O	64.951241000	60.275736000	33.913208000
O	65.064763000	58.138053000	35.414871000
O	64.961601000	57.871231000	32.959335000
Mg	65.878997000	62.165008000	34.219293000
O	69.065169000	67.525061000	35.892240000
H	68.274411000	67.904187000	36.415073000
H	69.512607000	66.962775000	36.543225000
C	64.858565000	58.296584000	31.582123000
H	65.810167000	58.708232000	31.240900000
H	64.592846000	57.403011000	31.013332000
H	64.066525000	59.045950000	31.485174000
C	66.126779000	51.982031000	31.695864000
H	66.441199000	52.268419000	30.686157000
H	67.031727000	51.870388000	32.304857000
H	65.646981000	50.997178000	31.630379000
C	70.162656000	56.391220000	33.158986000
H	70.175610000	56.106194000	32.100704000
H	70.322723000	55.503112000	33.773999000
H	69.189044000	56.832956000	33.401242000
C	72.624505000	58.656791000	35.017428000
H	72.287608000	58.887524000	36.035803000
H	73.699863000	58.465899000	35.053016000
C	73.032247000	61.736835000	32.780153000
H	73.060428000	62.636264000	33.404191000
H	73.802025000	61.823016000	32.009715000
C	70.034419000	60.698314000	30.637846000
H	70.027381000	60.819522000	29.548592000
H	69.657820000	59.703510000	30.869179000

H	69.371768000	61.435998000	31.089184000
C	68.291731000	60.164470000	40.471282000
H	67.836131000	59.425970000	39.805638000
H	68.029821000	59.909582000	41.505553000
H	67.866017000	61.141518000	40.230899000
C	64.938053000	67.198047000	39.416267000
H	65.933780000	66.984667000	39.820476000
H	64.262233000	67.393768000	40.257896000
H	64.583933000	66.295794000	38.902967000
C	62.363490000	66.368004000	31.201870000
H	61.720478000	65.691434000	30.626456000
H	61.933509000	66.463326000	32.205732000
H	62.313326000	67.356632000	30.727705000
C	61.830354000	64.128633000	34.247869000
H	61.806486000	63.105260000	34.630961000
H	60.809502000	64.530011000	34.276050000
H	62.149369000	64.081755000	33.205326000
C	63.637406000	60.372278000	37.385585000
H	62.957049000	59.711094000	37.936364000
H	63.254330000	61.394545000	37.464316000
H	63.626295000	60.090091000	36.333135000
H	70.045919000	61.960600000	37.624656000
H	67.918454000	61.590903000	36.977329000
O	65.891454000	62.299672000	32.109942000
H	66.485932000	61.515106000	31.888604000
H	65.004371000	62.022847000	31.833109000
<u>dissociative TS (-4395.571911 A.U.)</u>			
C	71.494702000	60.998930000	30.984056000
O	72.420952000	60.672987000	30.245128000
N	71.705704000	61.653948000	32.176270000
H	70.905166000	61.784601000	32.784118000
C	73.449953000	60.537842000	33.655407000
O	74.641717000	60.293843000	33.834677000
N	72.425307000	59.844329000	34.212338000
H	71.469418000	60.160165000	34.072823000
C	72.017811000	57.355044000	34.456489000
O	72.499650000	56.264518000	34.766941000
N	70.924768000	57.508546000	33.667222000
H	70.490393000	58.426228000	33.579054000
C	65.321766000	53.241511000	32.029055000
H	66.009711000	54.025769000	32.368647000
H	64.846186000	53.626450000	31.115259000
C	64.240861000	52.991481000	33.090779000
H	63.590606000	52.173650000	32.749151000

H	64.716097000	52.633408000	34.016071000
C	63.364580000	54.214011000	33.411823000
H	62.903214000	54.587458000	32.484812000
H	62.535861000	53.901975000	34.065025000
C	64.122169000	55.360206000	34.092147000
H	64.587262000	55.006702000	35.020231000
H	64.929751000	55.732107000	33.455839000
N	63.291542000	56.533103000	34.433945000
H	62.517648000	56.267244000	35.042125000
H	64.319629000	57.682631000	34.967555000
H	62.888834000	56.932778000	33.586968000
C	65.644735000	68.335114000	38.657110000
H	64.912460000	69.057262000	38.279965000
H	66.322954000	68.856379000	39.343548000
C	66.465371000	67.795593000	37.472481000
O	67.533159000	67.181057000	37.795150000
O	66.009967000	67.953883000	36.309298000
C	63.851004000	66.009956000	31.166665000
H	63.987185000	64.990362000	31.550302000
H	64.202672000	65.992034000	30.125414000
C	64.736929000	66.957282000	31.990317000
H	64.706114000	67.971137000	31.565467000
H	64.330632000	67.038001000	33.007701000
C	66.179192000	66.439650000	32.078580000
H	66.139182000	65.377619000	32.351068000
H	66.655598000	66.481102000	31.088380000
C	67.047597000	67.171269000	33.107943000
H	67.466462000	68.107498000	32.725889000
H	66.511097000	67.394919000	34.036271000
N	68.178922000	66.279261000	33.517118000
H	68.860163000	66.089547000	32.779358000
H	68.676739000	66.582128000	34.385816000
H	67.787727000	65.353454000	33.838613000
C	62.622999000	65.163663000	35.037267000
H	62.529225000	66.167985000	34.603397000
H	62.255958000	65.243473000	36.068643000
C	64.082768000	64.757405000	35.076639000
O	64.403151000	63.694412000	34.502542000
N	64.958431000	65.516472000	35.724140000
H	65.931628000	65.203531000	35.729222000
H	64.806013000	66.476663000	36.032091000
C	65.053521000	60.353725000	37.961378000
H	65.059957000	60.418957000	39.056754000
H	65.556654000	59.412348000	37.707998000

C	65.926820000	61.461856000	37.415315000
O	65.520969000	62.247477000	36.554550000
O	67.132196000	61.501242000	37.920677000
C	69.823959000	60.175505000	40.310931000
H	70.278189000	60.713442000	41.152395000
H	70.224204000	59.158123000	40.292163000
C	70.227850000	60.858319000	39.016578000
O	70.681159000	60.293422000	38.044558000
O	69.972041000	62.180173000	39.077916000
O	67.331390000	64.186463000	34.990889000
P	68.742874000	63.826242000	35.514786000
O	68.826251000	63.285743000	36.917304000
O	69.881027000	63.937457000	34.565110000
O	67.800163000	61.569173000	34.738419000
P	68.161830000	60.516502000	33.662786000
O	67.562357000	60.860853000	32.291667000
O	69.569774000	59.997883000	33.702291000
O	67.165308000	59.155922000	34.148573000
P	65.593294000	59.263352000	34.065850000
O	65.062210000	60.677639000	34.078213000
O	65.076051000	58.327493000	35.227727000
O	65.067137000	58.444293000	32.765536000
Mg	66.059809000	62.529553000	34.556840000
O	68.984029000	66.058769000	36.085997000
H	68.315241000	66.521577000	36.786799000
H	69.866134000	66.099933000	36.487996000
C	65.157343000	59.039284000	31.453432000
H	66.139726000	59.493675000	31.304669000
H	64.990955000	58.227671000	30.740938000
H	64.374471000	59.797039000	31.337056000
C	66.126779000	51.982031000	31.695864000
H	66.890528000	52.186738000	30.937632000
H	66.638666000	51.593619000	32.584693000
H	65.477747000	51.184730000	31.311703000
C	70.162655000	56.391220000	33.158985000
H	70.213279000	56.332486000	32.062506000
H	70.579100000	55.472880000	33.579758000
H	69.109133000	56.484893000	33.450866000
C	72.624506000	58.656791000	35.017429000
H	72.202538000	58.810785000	36.020594000
H	73.698539000	58.498483000	35.120275000
C	73.032248000	61.736835000	32.780153000
H	73.087013000	62.645643000	33.390651000
H	73.768163000	61.808696000	31.978741000

C	70.034419000	60.698315000	30.637845000
H	69.965197000	60.583407000	29.552560000
H	69.740466000	59.763876000	31.119584000
H	69.339979000	61.459512000	30.988078000
C	68.291732000	60.164471000	40.471281000
H	67.821072000	59.624611000	39.646268000
H	68.014307000	59.672184000	41.411945000
H	67.896528000	61.182081000	40.475544000
C	64.938053000	67.198047000	39.416267000
H	65.674289000	66.476346000	39.783387000
H	64.369818000	67.582786000	40.271928000
H	64.239258000	66.660496000	38.763502000
C	62.363490000	66.368004000	31.201870000
H	61.768442000	65.656046000	30.618078000
H	61.975957000	66.362643000	32.226675000
H	62.182944000	67.368320000	30.787366000
C	61.830354000	64.128633000	34.247869000
H	61.928007000	63.139497000	34.700354000
H	60.766742000	64.396697000	34.221220000
H	62.189568000	64.054510000	33.219107000
C	63.637404000	60.372277000	37.385585000
H	63.068741000	59.513290000	37.760472000
H	63.105795000	61.285802000	37.673582000
H	63.669038000	60.326036000	36.297037000
H	69.962387000	62.556948000	38.165307000
H	67.703586000	62.207186000	37.472769000
O	66.110714000	62.919521000	32.468429000
H	66.730573000	62.125959000	32.247385000
H	65.227243000	62.626531000	32.196012000
<u>dissociative Pr (-4395.627973 A.U.)</u>			
C	71.439798000	60.698646000	31.238746000
O	72.279364000	59.863143000	30.894248000
N	71.711970000	61.663092000	32.164237000
H	70.968042000	62.287596000	32.504664000
C	73.432547000	60.504089000	33.608422000
O	74.614164000	60.202665000	33.743581000
N	72.401632000	59.821991000	34.184820000
H	71.473740000	60.231359000	34.159367000
C	71.764692000	57.427681000	34.704777000
O	71.706252000	56.509705000	35.521167000
N	71.093527000	57.444073000	33.527565000
H	71.303333000	58.180631000	32.865121000
C	65.088329000	53.099723000	31.829220000
H	65.602194000	54.053963000	31.999658000

H	64.546564000	53.209059000	30.878145000
C	64.077405000	52.825421000	32.952523000
H	63.652946000	51.821213000	32.808794000
H	64.603116000	52.795758000	33.918383000
C	62.918889000	53.831667000	33.032367000
H	62.414794000	53.880433000	32.054661000
H	62.168076000	53.461188000	33.747336000
C	63.331493000	55.247132000	33.450827000
H	63.815221000	55.226742000	34.434427000
H	64.055554000	55.682280000	32.756516000
N	62.193253000	56.191170000	33.538341000
H	61.492457000	55.841690000	34.192545000
H	62.597027000	57.738412000	33.810906000
H	61.730509000	56.257676000	32.630552000
C	66.126015000	66.238711000	39.307004000
H	67.028272000	66.671990000	39.759126000
H	65.943982000	65.307686000	39.857490000
C	66.471855000	65.865148000	37.873497000
O	67.410966000	64.928043000	37.820252000
O	65.933818000	66.389554000	36.907066000
C	63.465376000	66.250729000	30.139309000
H	63.192267000	65.460769000	29.424451000
H	63.519868000	67.181017000	29.555319000
C	64.847598000	65.937402000	30.731794000
H	65.158952000	66.767113000	31.384591000
H	64.759619000	65.055776000	31.378649000
C	65.928126000	65.685781000	29.669015000
H	65.645069000	64.810630000	29.066300000
H	65.970457000	66.540145000	28.977837000
C	67.335708000	65.455640000	30.238302000
H	68.024486000	65.239329000	29.413461000
H	67.693042000	66.383354000	30.715727000
N	67.370306000	64.315949000	31.167504000
H	66.479097000	62.912262000	30.999865000
H	68.324788000	64.059273000	31.438600000
H	66.942695000	64.560205000	32.059447000
C	63.066333000	64.966207000	34.564441000
H	63.008299000	65.947474000	34.075545000
H	63.141216000	65.174065000	35.639479000
C	64.358478000	64.297625000	34.114696000
O	64.321119000	63.305367000	33.351566000
N	65.505964000	64.838333000	34.525148000
H	66.347303000	64.281539000	34.326602000
H	65.550014000	65.527003000	35.274131000

C	65.043486000	59.796736000	37.207056000
H	65.621368000	59.829223000	38.136829000
H	64.990025000	58.736666000	36.922597000
C	65.857599000	60.485643000	36.124962000
O	65.305912000	61.160487000	35.245133000
O	67.136634000	60.270011000	36.237236000
C	69.016070000	61.402389000	39.924759000
H	68.380044000	62.291670000	39.961865000
H	69.905021000	61.605115000	40.537477000
C	69.490129000	61.177354000	38.491307000
O	70.110929000	60.189994000	38.147800000
O	69.140729000	62.183828000	37.686283000
O	67.195931000	62.854338000	33.656489000
P	68.636676000	62.913105000	34.221349000
O	68.973446000	61.676628000	35.079175000
O	69.684082000	63.375293000	33.220036000
O	66.585066000	59.821022000	32.941167000
P	66.335751000	58.729373000	31.912356000
O	66.216396000	59.422888000	30.448829000
O	67.074215000	57.445969000	31.870385000
O	64.678966000	58.268671000	32.162571000
P	63.486819000	59.259898000	32.515619000
O	63.859841000	60.711013000	32.533241000
O	62.806897000	58.750709000	33.839334000
O	62.363722000	58.916385000	31.396216000
Mg	65.668581000	61.618283000	33.233761000
O	68.497330000	64.223528000	35.320512000
H	67.670667000	64.668614000	36.891893000
H	69.309535000	64.744297000	35.218007000
C	62.663634000	59.240262000	30.027482000
H	63.673303000	58.915860000	29.757203000
H	61.926391000	58.716232000	29.414630000
H	62.569505000	60.319786000	29.869491000
C	66.126779000	51.982031000	31.695864000
H	66.839615000	52.196678000	30.892291000
H	66.701311000	51.863466000	32.622631000
H	65.649013000	51.018540000	31.475026000
C	70.162653000	56.391218000	33.158985000
H	70.612638000	55.685331000	32.446071000
H	69.909407000	55.845267000	34.069335000
H	69.255162000	56.815695000	32.718967000
C	72.624507000	58.656793000	35.017428000
H	72.436879000	58.884157000	36.074089000
H	73.681117000	58.393155000	34.918024000

C	73.032248000	61.736835000	32.780155000
H	73.045072000	62.618596000	33.429478000
H	73.813698000	61.849662000	32.023202000
C	70.034418000	60.698313000	30.637845000
H	70.117334000	60.858726000	29.557439000
H	69.577513000	59.715358000	30.787733000
H	69.385180000	61.462281000	31.073997000
C	68.291731000	60.164470000	40.471282000
H	68.930811000	59.282824000	40.369318000
H	68.030686000	60.293721000	41.528248000
H	67.368046000	59.971969000	39.913498000
C	64.938053000	67.198047000	39.416267000
H	64.032262000	66.750429000	38.995283000
H	64.743485000	67.448167000	40.464846000
H	65.131130000	68.124004000	38.866842000
C	62.363490000	66.368004000	31.201870000
H	61.396565000	66.617326000	30.748266000
H	62.245742000	65.426627000	31.744918000
H	62.599417000	67.152797000	31.931498000
C	61.830354000	64.128633000	34.247869000
H	61.858595000	63.175175000	34.783991000
H	60.918567000	64.663838000	34.537576000
H	61.773625000	63.889473000	33.183932000
C	63.637406000	60.372278000	37.385585000
H	63.098252000	59.823478000	38.166388000
H	63.676164000	61.427651000	37.676700000
H	63.072887000	60.299663000	36.452203000
H	69.307532000	61.949934000	36.722750000
H	67.750132000	60.790863000	35.593183000
O	65.863742000	62.094812000	31.105868000
H	66.174932000	60.404028000	30.555415000
H	64.962239000	62.390676000	30.902438000

Energy corrections of reactants, transition structures and products

1. Model_{1-wat} for AceK

		E_{opt}	ΔE_{freq}	$\Delta E_{\text{basis set}}$	ΔE_{CPCM}	ΔE_{D2}	E_{correct}
associative	Re	-4126.553941	1.018049	-1.350113	-0.069784	-0.211226	-4127.167015
	TS	-4126.511088	1.014814	-1.352055	-0.071181	-0.206113	-4127.125624
	Pr	-4126.580031	1.019118	-1.352713	-0.074884	-0.203390	-4127.191900
dissociative	Re	-4126.535051	1.017648	-1.353783	-0.076600	-0.205684	-4127.153471
	TS	-4126.520042	1.016886	-1.350666	-0.078837	-0.205912	-4127.138570
	Pr	-4126.569152	1.017796	-1.356364	-0.080378	-0.193968	-4127.182066

2. Model_{2-wat} for AceK

		E_{opt}	ΔE_{freq}	$\Delta E_{\text{basis set}}$	ΔE_{CPCM}	ΔE_{D2}	E_{correct}
associative	Re	-4202.981235	1.046632	-1.397075	-0.077244	-0.209356	-4203.618278
	TS	-4202.923531	1.042836	-1.396180	-0.075797	-0.210317	-4203.562989
	Pr	-4202.996976	1.046910	-1.395400	-0.075377	-0.213185	-4203.634028
dissociative	Re	-4202.970481	1.046996	-1.392363	-0.076575	-0.216090	-4203.608513
	TS	-4202.936471	1.043389	-1.395292	-0.080744	-0.215252	-4203.584369
	Pr	-4202.963656	1.043444	-1.400138	-0.078808	-0.210679	-4203.609837

3. Two-lytic-water model for AceK

		E_{opt}	ΔE_{freq}	$\Delta E_{\text{basis set}}$	ΔE_{CPCM}	ΔE_{D2}	E_{correct}
associative	Re	-4202.986110	1.045435	-1.391619	-0.073387	-0.219608	-4203.625289
	TS	-4202.938312	1.042343	-1.389669	-0.071257	-0.218661	-4203.575555
	Pr	-4203.028345	1.046283	-1.392196	-0.075710	-0.211472	-4203.661440
dissociative	Re	-4202.985920	1.046214	-1.391519	-0.072069	-0.218739	-4203.622033
	TS	-4202.948299	1.044330	-1.393226	-0.076207	-0.217887	-4203.591290
	Pr	-4203.014493	1.044352	-1.397709	-0.073434	-0.203872	-4203.645155

4. Double Mg²⁺ model for AceK

		E _{opt}	ΔE _{freq}	ΔE _{basis set}	ΔE _{CPCM}	ΔE _{D2}	E _{correct}
	Re	-4555.828934	1.102274	-1.468669	-0.085336	-0.234650	-4556.515315
associative	TS	-4555.772486	1.099608	-1.466398	-0.085074	-0.237116	-4556.461466
	Pr	-4555.846460	1.100496	-1.469561	-0.089984	-0.233309	-4556.538818
	Re	-4555.854524	1.105563	-1.462466	-0.076545	-0.246649	-4556.534621
dissociative	TS	-4555.806619	1.101817	-1.461849	-0.076148	-0.245356	-4556.488156
	Pr	-4555.866443	1.102070	-1.466821	-0.080396	-0.230050	-4556.541640

5. Model for AceK-ICDH

		E _{opt}	ΔE _{freq}	ΔE _{basis set}	ΔE _{CPCM}	ΔE _{D2}	E _{correct}
	Re	-4394.953321	1.111220	-1.458405	-0.077742	-0.225801	-4395.604049
associative	TS	-4394.910198	1.109544	-1.460130	-0.077234	-0.222516	-4395.560534
	Pr	-4394.983287	1.113288	-1.457886	-0.077118	-0.222028	-4395.627029
	Re	-4394.952559	1.112495	-1.461792	-0.081801	-0.222798	-4395.606456
dissociative	TS	-4394.917190	1.111231	-1.459596	-0.083895	-0.222461	-4395.571911
	Pr	-4394.982817	1.109172	-1.465105	-0.080869	-0.208354	-4395.627973