Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information (ESI)

Probing the Early Stages of Solvation of *cis*-Pinate Dianion by Water, Acetonitrile, and Methanol: A Photoelectron Spectroscopy and Theoretical Study

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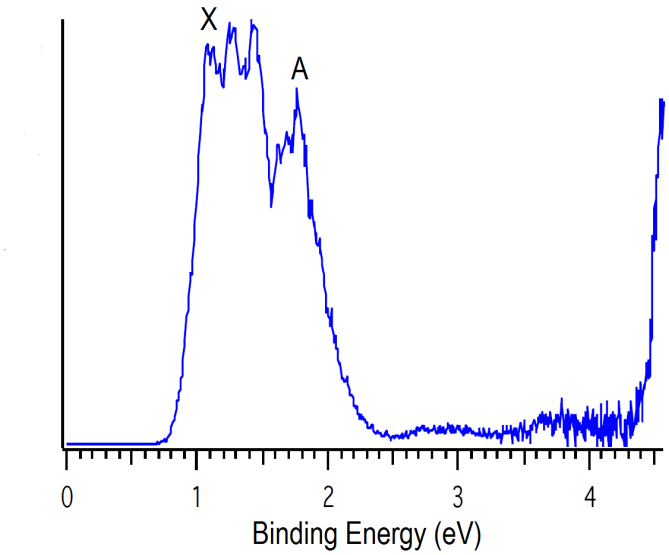

Figure S1. The 20 K photoelectron spectrum of bare *cis*-PA^{2-} at 266 nm.

Table S1. Comparison of experimental VDE value to calculated ones for the bare *cis*-PA^{2-} dianion at different theoretical levels.

Methods	EBE (eV)
Experiment	1.15 ± 0.05
M06-2X/aug-cc-pVDZ	1.15
M06-2X/6-311++G(d,p)	1.22
ωB97X-D/aug-cc-pVDZ	1.14
ωB97X-D/6-311++G(d,p)	1.16
B3LYP/aug-cc-pVDZ	0.55
B3LYP/6-311++G(d,p)	0.58
BHLYP/aug-cc-pVDZ	1.05
BLYP/aug-cc-pVDZ	-0.13
BP86/aug-cc-pVDZ	0.13
PBE/aug-cc-pVDZ	-0.03
PW91/aug-cc-pVDZ	0.03
TPSS/aug-cc-pVDZ	-0.12
MP2/aug-cc-pVDZ	0.76
MP2/6-311++G(d,p)	0.63

Table S2. Comparison of experimental VDEs to calculated ones and the relative energies (ΔE) of different isomers for the solvated *cis*-PA^{2-} clusters at different theoretical levels. The aug-cc-pVDZ basis set was used for all the calculations.

Clusters	Isomers	ΔE (kJ/mol)		EBE (eV)	
		M06-2X	MP2//M06-2X	Calc.(M06-2X)	Exp.
cis-$PA^{2-}(H_2O)$	iso A	0.00	0.00	1.57	1.43± 0.05
	iso B	0.25	0.05	1.49	
	iso C	15.65	15.51	1.47	
	iso D	15.66	15.67	1.52	
cis-$PA^{2-}(H_2O)_2$	iso A	0.00	0.00	2.13	2.07 ± 0.10
	iso B	15.55	15.30	2.14	
	iso C	15.68	15.05	2.07	
	iso D	18.91	17.00	1.56	1.45 ± 0.05
	iso E	19.97	19.25	1.65	
cis-$PA^{2-}(H_2O)_3$	iso A	0.00	0.00	2.28	2.30 ± 0.05
	iso B	0.48	1.82	2.42	
	iso C	1.54	2.38	2.38	
	iso D	19.79	18.51	1.84	
	iso E	19.86	16.34	1.65	
cis-$PA^{2-}(H_2O)_4$	iso A	0.00	1.65	2.72	2.75 ± 0.10
	iso B	0.32	0.00	2.50	
	iso C	0.36	1.84	2.53	
	iso D	27.45	23.13	1.93	
	iso E	28.38	22.84	1.84	
	iso B	0.32	0.00	2.50	
cis-$PA^{2-}(CH_3CN)$	iso A	0.00	0.01	1.60	1.44± 0.05
	iso B	2.55	0.00	1.53	
cis-$PA^{2-}(CH_3CN)_2$	iso A	0.00	0.00	2.12	2.08 ± 0.05
	iso B	22.40	11.00	1.74	
cis-$PA^{2-}(CH_3OH)$	iso A	0.00	0.34	1.61	1.44 ± 0.05
	iso B	0.38	0.00	1.53	
cis-$PA^{2-}(CH_3OH)_2$	iso A	0.00	0.00	2.29	2.10 ± 0.10
	iso B	20.62	13.71	1.67	1.60 ± 0.10
cis-$PA^{2-}(CH_3CN)(H_2O)$	iso A	0.00	0.00	2.12	2.07 ± 0.05
	iso B	0.48	0.20	2.11	
	iso C	7.81	4.70	1.73	1.50 ± 0.10
	iso D	51.66	49.34	1.61	
cis-$PA^{2-}(CH_3CN)(H_2O)_2$	iso A	0.00	0.12	2.44	2.29± 0.05
	iso B	2.11	0.00	2.35	
	iso C	11.72	14.03	2.29	
	iso D	27.85	22.10	1.83	1.60± 0.10
cis-$PA^{2-}(CH_3OH)(H_2O)$	iso A	0.00	0.00	2.20	2.08 ± 0.05
	iso B	2.63	1.14	2.12	
	iso C	23.50	19.22	1.65	

Cartesian coordinates and energies for all isomers optimized at the M06-2X/aug-cc-pVDZ level of theory:

Cluster: *cis*-PA^{2-}

Sum of electronic and zero-point Energies = -650.752343

C	0.65071800	0.86560300	0.03222800
C	1.39302100	-0.29408500	-0.69984700
C	0.11164000	-1.14220400	-0.55704000
C	-0.69010800	0.16553600	-0.34968400
C	0.88007000	2.26521400	-0.51613600
C	0.93701900	0.83728300	1.53134400
C	2.75330300	-0.72678200	-0.11181100
C	-1.88255100	0.21485100	0.58962300
C	-3.25199100	-0.24284300	-0.00379700
O	2.81944000	-1.84294300	0.45775300
O	3.67315800	0.12826100	-0.24595100
O	-3.37626100	-0.21145900	-1.25276300
O	-4.12333500	-0.55942100	0.84895900
H	0.16608600	-1.75113100	0.35437800
H	-0.18324300	-1.78136500	-1.39777700
H	0.82015100	-0.17514700	1.93678000
H	1.97571800	1.14900500	1.71006800
H	0.25407700	1.51110900	2.07099600
H	0.23662700	3.00029300	-0.00423500
H	1.93387400	2.54747800	-0.37585600
H	0.64958800	2.29702900	-1.59042100
H	-1.01731500	0.53873200	-1.32993400
H	1.55192400	0.00443900	-1.74707000
H	-1.69532000	-0.36920900	1.50143600
H	-2.04291300	1.25782200	0.91836800

Cluster: *cis*-$PA^{2-}(H_2O)$

Isomer: iso A

Sum of electronic and zero-point Energies = -727.172894

C	1.25850000	0.86846300	-0.03234900
C	1.89041100	-0.38390200	-0.71428500
C	0.57960700	-1.14506500	-0.42567500
C	-0.13753900	0.21759300	-0.27322300
C	1.52174700	2.20663900	-0.70388300
C	1.63942600	0.93808700	1.44453700

C	3.25785400	-0.84625400	-0.16585400
C	-1.25396500	0.40759800	0.73928000
C	-2.67623000	0.00111500	0.28009900
O	3.28977800	-1.89939000	0.51465900
O	4.21572900	-0.07126900	-0.44091600
O	-2.90207700	-0.05035000	-0.95685000
O	-3.51067000	-0.19921700	1.20724900
H	0.66674400	-1.68281700	0.52681000
H	0.19671700	-1.83080100	-1.19058100
H	1.50871000	-0.03511100	1.93360100
H	2.69948900	1.21274900	1.53485900
H	1.02358900	1.68275300	1.97145600
H	0.95972000	3.01573500	-0.20863700
H	2.59651800	2.43415800	-0.65875600
H	1.21695100	2.17216900	-1.75921200
H	-0.50924700	0.53725600	-1.25608600
H	2.00045700	-0.17681900	-1.78899500
H	-1.03807700	-0.12265500	1.67648300
H	-1.33055700	1.47789600	1.00118100
O	-5.64812600	-0.46621800	-0.55995500
H	-4.83766100	-0.34556700	-1.09167000
H	-5.18929600	-0.43303600	0.30416000

Cluster: *cis*-$PA^{2-}(H_2O)$

Isomer: iso B

Sum of electronic and zero-point Energies = -727.172800

C	0.03960400	1.01076700	0.09994400
C	0.84810000	0.05534600	-0.83198700
C	-0.32790400	-0.93919500	-0.75694000
C	-1.24305700	0.23209900	-0.32637000
C	0.09366400	2.49106200	-0.24178200
C	0.41138200	0.79373700	1.56435600
C	2.26846300	-0.30553900	-0.37933600
C	-2.37891600	0.01684400	0.65675600
C	-3.72107400	-0.50243700	0.05094700
O	2.47973400	-1.46052200	0.07013600
O	3.11211500	0.63532700	-0.47556000
O	-3.90641200	-0.31103900	-1.17589400
O	-4.50967900	-1.02847300	0.87836100
H	-0.16148000	-1.65922000	0.05380200
H	-0.60365500	-1.48258600	-1.66785500
H	0.42632000	-0.27367400	1.81552300
H	1.41663400	1.19555500	1.75411800
H	-0.31054700	1.29665100	2.22466800

H	-0.59566700	3.06632600	0.39764400
H	1.11569500	2.87101400	-0.09911600
H	-0.19550800	2.65265800	-1.28960200
H	-1.66081400	0.70227900	-1.22721600
H	0.91426300	0.51658800	-1.82775200
H	-2.08394600	-0.66614400	1.46541300
H	-2.62942100	0.97875200	1.13943700
O	5.22894200	-0.92146500	0.41568800
H	4.74960800	-0.13304200	0.08475100
H	4.43934700	-1.49188000	0.46081800

Cluster: *cis*-$PA^{2-}(H_2O)$

Isomer: iso C

Sum of electronic and zero-point Energies = -727.166932

C	0.10136700	0.84179000	0.00273500
C	0.80312500	-0.34294000	-0.73104000
C	-0.49318100	-1.15973200	-0.55806000
C	-1.26040600	0.16814600	-0.35166600
C	0.34937000	2.23019200	-0.56496700
C	0.40757900	0.82245800	1.49781600
C	2.14949000	-0.80921000	-0.15871500
C	-2.43638500	0.25204400	0.60401500
C	-3.81887900	-0.19554200	0.03240400
O	2.20590400	-1.88627600	0.46236500
O	3.10560800	0.01028400	-0.36270500
O	-3.94112800	-0.22196700	-1.21665600
O	-4.69524900	-0.44793300	0.89972800
H	-0.43942200	-1.75986100	0.35890200
H	-0.81544900	-1.79918500	-1.38774500
H	0.27973200	-0.18318900	1.91599800
H	1.45154600	1.12244200	1.66606000
H	-0.25899700	1.51141500	2.03758800
H	-0.28049500	2.97875700	-0.05694200
H	1.40656400	2.50429200	-0.43543800
H	0.11124200	2.25305600	-1.63750800
H	-1.59412400	0.53758700	-1.33096400
H	0.95596000	-0.05840100	-1.78217000
H	-2.24646700	-0.32225500	1.52151100
H	-2.57580200	1.30149000	0.92020500
O	5.67340000	0.07458600	0.17738500
H	4.69516300	-0.13001300	0.06069400
H	5.70978300	0.97107800	-0.16626000

Cluster: *cis*-$PA^{2-}(H_2O)$

Isomer: iso D

Sum of electronic and zero-point Energies = -727.166931

C	-1.21921100	0.72766400	0.48527100
C	-1.75587000	-0.73570800	0.43009200
C	-0.48286500	-1.12442800	-0.35066400
C	0.20083100	0.15084600	0.19820500
C	-1.41036300	1.46834700	1.79910400
C	-1.77469900	1.55656500	-0.67003400
C	-3.17588900	-0.92602900	-0.14589900
C	1.18670400	0.93808600	-0.64848000
C	2.65325700	0.43489300	-0.65426100
O	-3.28374300	-1.46600600	-1.27282200
O	-4.09772400	-0.47373500	0.58875900
O	3.04176200	-0.18381100	0.38321800
O	3.34063800	0.72570100	-1.65469700
H	-0.67685600	-1.06677400	-1.42893600
H	-0.00822400	-2.08671100	-0.12436200
H	-1.69571200	1.01432800	-1.62035100
H	-2.84000400	1.75782900	-0.49240300
H	-1.23262900	2.51000100	-0.76279600
H	-0.90988800	2.45075700	1.77518200
H	-2.48398300	1.61489300	1.98556900
H	-0.98740600	0.88816900	2.63134900
H	0.68380900	-0.08501600	1.15616000
H	-1.73703300	-1.15136100	1.44861700
H	0.84935400	1.00565500	-1.69106700
H	1.23913300	1.97396200	-0.26801600
O	5.36915300	-1.24076100	1.02174500
H	4.57659100	-0.75148200	0.64356700
H	4.93078800	-1.90677300	1.55786200

Cluster: *cis*-$PA^{2-}(H_2O)_2$

Isomer: iso A

Sum of electronic and zero-point Energies = -803.592705

C	0.66261000	1.08375100	0.00768800
C	1.36292700	-0.03069800	-0.82998300
C	0.13203200	-0.92700000	-0.58593200
C	-0.68385900	0.34783900	-0.26538900
C	0.78849900	2.50446700	-0.51826400
C	1.09388900	1.02333700	1.47079000
C	2.77454600	-0.43450500	-0.38593900
C	-1.77637300	0.33363100	0.78757300
C	-3.16978900	-0.15256500	0.31594500
O	2.92812500	-1.54868400	0.17467800

O	3.66873900	0.43476900	-0.60650500
O	-3.40136000	-0.15989500	-0.92008800
O	-3.97497000	-0.46299300	1.23818600
H	0.29586100	-1.55349900	0.29946700
H	-0.22242000	-1.55551000	-1.41042500
H	1.05373800	-0.00274900	1.85637000
H	2.13192800	1.37149400	1.56290700
H	0.44401400	1.65592100	2.09318100
H	0.16696600	3.19709600	0.07219900
H	1.83714400	2.83044000	-0.46562800
H	0.45987600	2.55589500	-1.56547700
H	-1.11270500	0.73576800	-1.19895700
H	1.41330200	0.30004200	-1.87712100
H	-1.48609700	-0.27050700	1.65768500
H	-1.93686600	1.35865100	1.16501600
O	-6.11081000	-0.81207800	-0.51274100
H	-5.33075600	-0.60832700	-1.06174900
H	-5.63120500	-0.77860000	0.34031600
O	5.71898100	-1.16077100	0.38406900
H	5.28417200	-0.37890600	-0.01446400
H	4.89650300	-1.66952200	0.50694000

Cluster: *cis*-$PA^{2-}(H_2O)_2$

Isomer: iso B

Sum of electronic and zero-point Energies = -803.586783

C	0.73935900	1.08099200	0.19129100
C	1.48711300	0.17467300	-0.83559900
C	0.21408900	-0.69011900	-0.93214100
C	-0.59383500	0.50654800	-0.37639000
C	0.95845200	2.57887500	0.05473100
C	1.02150800	0.63404100	1.62340400
C	2.83824400	-0.39562700	-0.38563900
C	-1.78669400	0.28978800	0.53567000
C	-3.13757400	0.01266600	-0.17441800
O	2.90671900	-1.61862600	-0.10424400
O	3.77346700	0.45518600	-0.30797900
O	-3.24897000	0.30740500	-1.37857200
O	-4.03727900	-0.46755800	0.58478600
H	0.27305100	-1.52286500	-0.22056000
H	-0.07595800	-1.07701100	-1.91537200
H	0.91601500	-0.45265900	1.72857000
H	2.05409900	0.89400500	1.89446800
H	0.32884800	1.12146700	2.32527400
H	0.30241600	3.13654300	0.74284700

H	2.00592100	2.82482400	0.28066600
H	0.73724000	2.90575200	-0.97080200
H	-0.91702700	1.13362300	-1.21831700
H	1.64727600	0.75169700	-1.75754300
H	-1.60331200	-0.52579200	1.24832600
H	-1.95540500	1.19578400	1.14407500
O	-6.57458200	-1.09461800	0.30344000
H	-5.62044100	-0.78855900	0.22425600
H	-6.54513100	-1.55904200	1.14396900
O	5.66691700	-1.42286900	0.46929600
H	5.29160000	-0.55070000	0.22755300
H	4.82667200	-1.90943400	0.38332000

Cluster: *cis*-$PA^{2-}(H_2O)_2$

Isomer: iso C

Sum of electronic and zero-point Energies = -803.586731

C	0.68690300	0.89213200	-0.01916800
C	1.32152400	-0.37332300	-0.67499800
C	0.00985900	-1.12891300	-0.38286700
C	-0.70668600	0.23686900	-0.26243700
C	0.95330500	2.21814900	-0.71264800
C	1.05200300	0.98710900	1.45994100
C	2.67188700	-0.83676400	-0.10899400
C	-1.83346900	0.44209400	0.73387200
C	-3.24388000	0.00440000	0.26538200
O	2.71212300	-1.85959100	0.59826500
O	3.64470600	-0.07002800	-0.41046300
O	-3.44210900	-0.10495600	-0.97208900
O	-4.09320100	-0.16227900	1.18453200
H	0.08650700	-1.64781100	0.58068500
H	-0.36581900	-1.82794900	-1.13843300
H	0.91637200	0.02278900	1.96466100
H	2.10925500	1.26847500	1.56208300
H	0.42764400	1.73845300	1.96576400
H	0.37421100	3.02999500	-0.24320000
H	2.02388900	2.46109800	-0.65241500
H	0.66786400	2.16107300	-1.77219000
H	-1.06816400	0.53731500	-1.25504300
H	1.44289600	-0.18514000	-1.75129100
H	-1.62291200	-0.06243200	1.68643900
H	-1.92538300	1.51744300	0.96752200
O	-6.19666600	-0.53576100	-0.60511400
H	-5.38323500	-0.43004700	-1.13395500
H	-5.74964400	-0.45718400	0.26203100

O	6.25082100	-0.15894800	-0.06545200
H	6.33801600	0.64374700	-0.58624000
H	5.25445100	-0.28784100	-0.08235100

Cluster: *cis*-$PA^{2-}(H_2O)_2$

Isomer: iso D

Sum of electronic and zero-point Energies = -803.585501

O	4.40416200	1.04660600	0.23892100
O	4.25291400	-1.18459300	0.57295300
C	3.86613900	-0.08482000	0.10560700
C	2.55685300	-0.08236900	-0.71453000
C	1.74858600	-1.37649300	-0.92671000
C	1.29067600	0.54849200	-0.04950800
H	2.74483200	0.43460300	-1.66702900
C	0.44588000	-0.56329700	-0.74754500
H	1.93663600	-2.06278700	-0.09115800
H	1.88322900	-1.92173600	-1.87150800
H	0.10360600	-0.16908200	-1.71383500
C	0.97740900	1.98516600	-0.43341000
H	0.01272800	2.30164600	-0.01261900
H	1.78072800	2.64294100	-0.07084100
H	0.91356500	2.08150900	-1.52631600
C	1.32949700	0.40056600	1.46776400
H	1.61582200	-0.61729200	1.76187500
H	2.08387900	1.08526900	1.87776600
H	0.34689100	0.63459000	1.90359100
C	-0.73267800	-1.21219200	-0.04227400
H	-0.46837500	-1.51620100	0.97886500
H	-0.99743000	-2.14177900	-0.57421600
C	-2.03079000	-0.38767800	0.02768300
O	-2.18013500	0.54746900	-0.80202800
O	-2.87342200	-0.74164400	0.90303500
O	-4.43398700	1.69985900	0.10597100
H	-4.33487200	1.17085900	0.90933800
H	-3.62102300	1.38162900	-0.37105500
O	-5.49750000	-1.04787000	0.01569900
H	-4.57464200	-1.10063100	0.34757500
H	-5.51127200	-0.12640100	-0.27930200

Cluster: *cis*-$PA^{2-}(H_2O)_2$

Isomer: iso E

Sum of electronic and zero-point Energies = -803.585097

O	2.67443900	0.72490600	-0.14754700
O	2.03315700	-1.43123800	-0.17260100

O	4.39758300	-1.37910100	1.11352100
H	4.27034400	-0.42483200	1.20646900
H	3.55702200	-1.58372200	0.62403400
H	5.33037800	-0.48899000	-0.62050300
O	5.25057200	0.32298700	-1.14023900
H	4.33085200	0.57780200	-0.90875200
C	1.82687100	-0.20043400	-0.33233700
C	0.42813400	0.26276900	-0.73550300
C	-0.74124300	-0.71948300	-0.94581200
C	-0.41652900	0.96264700	0.37584300
H	0.52867100	0.95378200	-1.58386900
C	-1.67786300	0.30922700	-0.26834300
H	-0.59483700	-1.61826100	-0.33411300
H	-0.98364800	-1.01784600	-1.97175000
H	-2.07314600	0.98646500	-1.03736200
C	-0.36826400	2.48155500	0.40408100
H	-1.09350100	2.87982000	1.13160600
H	0.63970200	2.82271100	0.68103800
H	-0.61579700	2.89098500	-0.58492400
C	-0.09056000	0.39852900	1.75595000
H	-0.08091700	-0.69805400	1.74678900
H	0.90499200	0.73968500	2.07314900
H	-0.83598000	0.73241900	2.49208600
C	-2.84070000	-0.14427600	0.59412000
H	-3.10945100	0.66307700	1.29844600
H	-2.56850100	-1.01337000	1.20853600
C	-4.16032300	-0.48497400	-0.16856800
O	-4.30117200	0.01002800	-1.31319800
O	-4.97499200	-1.19696200	0.47288100

Cluster: *cis*-$PA^{2-}(H_2O)_3$

Isomer: iso A

Sum of electronic and zero-point Energies = -880.004947

O	3.91529500	1.02055800	-0.23453400
O	3.75487600	-1.17022300	0.28316100
C	3.33855400	-0.10401800	-0.24111000
C	1.97806000	-0.13667900	-0.95102000
C	1.15033700	-1.43258700	-1.01417400
C	0.77059100	0.55249100	-0.23515100
H	2.09928300	0.31607500	-1.94517300
C	-0.13039800	-0.59485200	-0.79245800
H	1.39250900	-2.06277500	-0.14960500
H	1.21260000	-2.04109100	-1.92648800
H	-0.53993200	-0.25935100	-1.75477200

C	0.44317300	1.96399200	-0.69247700
H	-0.48843700	2.31483000	-0.22919500
H	1.27454100	2.63479100	-0.43135100
H	0.30435800	1.98831500	-1.78227700
C	0.91875600	0.50623000	1.28157800
H	1.21623200	-0.49203500	1.62715000
H	1.70281600	1.20915300	1.59354200
H	-0.02913400	0.78199000	1.76576100
C	-1.25181600	-1.19132300	0.03737000
H	-0.90886300	-1.43457700	1.05225700
H	-1.55885500	-2.15223500	-0.40741500
C	-2.53610200	-0.35293000	0.16553000
O	-2.65143200	0.66703200	-0.56210100
O	-3.39579800	-0.77841200	0.99094400
O	-4.96941400	1.67104800	0.40550200
H	-4.85806800	1.04048100	1.13112500
H	-4.14123200	1.44836900	-0.09251600
O	-5.98103800	-1.06798000	-0.03776800
H	-5.07310600	-1.14552100	0.32467200
H	-6.00299000	-0.11797800	-0.22019500
O	6.21632100	0.00269700	0.97922200
H	5.56763900	-0.72405700	0.92561200
H	5.63322800	0.67590600	0.57493100

Cluster: *cis*-$PA^{2-}(H_2O)_3$

Isomer: iso B

Sum of electronic and zero-point Energies = -880.004766

O	4.09841100	0.52674400	-0.62633900
O	3.33999100	-1.54343300	-0.14230800
O	-5.43175800	-1.73838600	-0.17178500
H	-4.97453200	-1.48455500	-0.98397000
H	-4.73236300	-1.46784300	0.48847600
H	-4.68171200	0.90493500	-0.85039100
O	-5.64028900	1.11146000	-0.85704300
H	-5.98612600	0.29881700	-0.46119800
C	3.19410700	-0.35169600	-0.51355500
C	1.77671100	0.14373000	-0.82826000
C	0.53969800	-0.76952400	-0.71574300
C	1.12486700	1.08580500	0.23164100
H	1.80027300	0.66759000	-1.79416900
C	-0.24213900	0.42784600	-0.12478500
H	0.72131000	-1.55764800	0.02521600
H	0.14679400	-1.22183200	-1.63322500
H	-0.70468900	0.99443300	-0.94366700

C	1.25857300	2.57813700	-0.02332900
H	0.67644800	3.15745000	0.71148300
H	2.31560500	2.87227200	0.04496900
H	0.89147900	2.83008400	-1.02779600
C	1.60506500	0.74385300	1.63926900
H	1.55416400	-0.33551300	1.82584700
H	2.65383700	1.05012500	1.75363700
H	0.99460600	1.26023100	2.39480000
C	-1.28524600	0.21241800	0.95733500
H	-1.46183100	1.16433400	1.48789800
H	-0.93788900	-0.50760900	1.70876000
C	-2.67226100	-0.24344900	0.46341700
O	-3.02882800	0.09586600	-0.69629200
O	-3.36786100	-0.89706800	1.29020700
O	6.14252800	-1.23656500	0.05677800
H	5.71940600	-0.39500000	-0.20942100
H	5.31143500	-1.74193800	0.12105600

Cluster: *cis*-$PA^{2-}(H_2O)_3$

Isomer: iso C

Sum of electronic and zero-point Energies = -880.004362

O	3.23341300	0.55193200	-0.42010400
O	2.47755500	-1.45585800	0.25967700
O	4.93733100	-1.13671200	1.34259500
H	4.84000000	-0.20311900	1.10764400
H	4.06362400	-1.45419500	0.99874700
H	5.78857900	-0.92691800	-0.64161900
O	5.69875700	-0.33153200	-1.39859800
H	4.81433300	0.04815200	-1.20752200
C	2.33007800	-0.32589400	-0.27075700
C	0.93601800	0.08461300	-0.74206300
C	-0.28794700	-0.84149200	-0.59917600
C	0.19154700	1.13414900	0.14215200
H	1.02143300	0.48343000	-1.76198500
C	-1.13309000	0.39897800	-0.22451100
H	-0.14815800	-1.52267400	0.24879200
H	-0.60281600	-1.41787200	-1.47570900
H	-1.53987600	0.84008900	-1.14420100
C	0.31299200	2.58657400	-0.28851600
H	-0.33965700	3.23022600	0.32259300
H	1.35277500	2.92585900	-0.17807600
H	0.01910900	2.70025700	-1.34094200
C	0.57134300	0.98440000	1.61284800
H	0.53799400	-0.06522900	1.92870100

H	1.59663800	1.34762500	1.76918100
H	-0.11346800	1.56271900	2.24977400
C	-2.25643900	0.29835100	0.78993600
H	-2.45691500	1.29697600	1.21603900
H	-1.97797300	-0.34594700	1.63466300
C	-3.61889400	-0.19604900	0.24169000
O	-3.81590100	-0.10818100	-0.99723100
O	-4.43471900	-0.60855200	1.11171200
O	-6.51414200	-0.87825900	-0.72379900
H	-6.05806900	-0.90356500	0.14198400
H	-5.72955100	-0.60029700	-1.23169400

Cluster: *cis*-$PA^{2-}(H_2O)_3$

Isomer: iso D

Sum of electronic and zero-point Energies = -879.997409

O	1.93949200	-0.21821800	1.03770900
O	2.67747600	0.15550900	-1.04917400
O	5.19643000	1.25079900	-0.67910300
H	5.54065300	0.36361300	-0.86080800
H	4.23604400	1.07581000	-0.79478200
H	4.86148800	0.40350400	1.24564500
O	4.53106200	-0.31477400	1.80508800
H	3.56340800	-0.32142500	1.57856100
O	4.82270400	-1.65229400	-0.73891000
H	4.84593700	-1.51133900	0.22300000
H	4.00067100	-1.16734300	-0.96646700
C	1.76732700	0.09872300	-0.16142000
C	0.36004500	0.50158500	-0.63055600
H	0.42521000	1.58128300	-0.84868300
H	0.18253400	0.01304700	-1.59830800
C	-0.77981000	0.23883100	0.33758400
C	-1.47232400	-1.14272200	0.40101100
C	-2.17781100	0.87478700	0.07439500
H	-0.45250600	0.51952100	1.34777300
C	-2.80787100	-0.41963000	0.67360200
H	-1.10174000	-1.85462300	1.14712800
H	-1.51509900	-1.63727000	-0.57758700
H	-2.96497100	-0.26596700	1.75127400
C	-4.14091100	-0.87993100	0.04433600
O	-4.12254700	-1.90737700	-0.67361300
O	-5.11960600	-0.12594300	0.30025400
C	-2.50687000	1.00347700	-1.41094600
H	-3.57062900	1.25226800	-1.52522200
H	-1.89600700	1.78840400	-1.88227500

H	-2.33370800	0.05719300	-1.93824800
C	-2.49145300	2.17528800	0.79571600
H	-1.92912300	3.01740200	0.35924700
H	-3.56809400	2.38363000	0.71997800
H	-2.22608200	2.09822800	1.85942500

Cluster: *cis*-$PA^{2-}(H_2O)_3$

Isomer: iso E

Sum of electronic and zero-point Energies = -879.997384

O	2.07588800	1.41810100	-0.24025400
O	2.00997700	-0.82601000	-0.32925800
O	4.65605100	-1.52589900	-0.81458600
H	4.73848800	-1.65192800	0.14263000
H	3.70600000	-1.28072200	-0.86307800
H	4.92138200	0.51482800	-0.27079700
O	4.70428600	1.27728200	0.28574900
H	3.72924600	1.38748800	0.11090600
O	3.77184600	-0.93000600	1.90696800
H	4.16366200	-0.07216900	1.66948700
H	3.01810800	-0.96177000	1.28214000
C	1.50819000	0.32555200	-0.50352000
C	0.08746500	0.42065500	-1.04917800
C	-0.68670100	-0.83388200	-1.48943200
C	-1.06373400	0.72087800	-0.03058500
H	0.07196700	1.19848100	-1.82439200
C	-1.97236100	-0.21612600	-0.88780500
H	-0.34223500	-1.70445700	-0.91850100
H	-0.68546800	-1.08598100	-2.55867300
H	-2.47758000	0.41245600	-1.63383200
C	-1.50013000	2.17127800	0.08531800
H	-2.42719400	2.23280500	0.66928200
H	-0.70347000	2.76852900	0.55369700
H	-1.70849500	2.58621600	-0.91084800
C	-0.75730100	0.14487300	1.34754100
H	-0.40338700	-0.89185300	1.28377300
H	0.03269900	0.73665100	1.83083400
H	-1.66004500	0.16865800	1.97310200
C	-2.99832700	-1.12365800	-0.23663800
H	-2.54673800	-1.70224000	0.58183300
H	-3.33856900	-1.86912600	-0.97512000
C	-4.28021700	-0.43154000	0.31497100
O	-4.44060600	0.78087400	0.02717300
O	-5.04115100	-1.17609800	0.98339800

Cluster: *cis*-$PA^{2-}(H_2O)_4$

Isomer: iso A

Sum of electronic and zero-point Energies = -956.416423

O	3.49973700	0.90547800	-0.08469400
O	3.25143200	-1.31848100	0.15147700
O	5.37044600	-0.64191800	1.67959200
H	5.07150700	0.27516700	1.60862000
H	4.65161200	-1.06524000	1.14143300
H	6.35660400	0.12389100	-0.07581300
O	6.21882500	0.80800800	-0.74609300
H	5.25201700	0.94247900	-0.65059800
C	2.87577000	-0.18418700	-0.24552800
C	1.52666000	-0.07836700	-0.95542800
C	0.67262800	-1.33011200	-1.22248800
C	0.33150700	0.51321600	-0.13666500
H	1.66038400	0.52428800	-1.86393100
C	-0.59009400	-0.50739000	-0.87515300
H	0.89051300	-2.09382200	-0.46604500
H	0.73041800	-1.78831900	-2.21861100
H	-0.98249800	-0.01257600	-1.77368000
C	0.03433700	1.98648500	-0.35675100
H	-0.89516500	2.26754700	0.15493900
H	0.87335200	2.59253900	0.01480900
H	-0.09859600	2.19287300	-1.42761800
C	0.47166700	0.21513700	1.35192300
H	0.74028600	-0.83370900	1.53066800
H	1.27049300	0.83794800	1.77696500
H	-0.47053000	0.43412500	1.87365300
C	-1.73269200	-1.19977200	-0.15603000
H	-1.40205400	-1.61243700	0.80714400
H	-2.06230500	-2.06698900	-0.75080400
C	-2.99114400	-0.35265100	0.10406200
O	-3.05535600	0.78607800	-0.42774600
O	-3.87966200	-0.88776800	0.82758700
O	-5.37027000	1.68291900	0.64360000
H	-5.30359700	0.93941600	1.25898300
H	-4.53441600	1.51522400	0.13655700
O	-6.45320300	-0.90129700	-0.28198800
H	-6.43604500	0.06610100	-0.29810300
H	-5.55939300	-1.07681300	0.07989800

Cluster: *cis*-$PA^{2-}(H_2O)_4$

Isomer: iso B

Sum of electronic and zero-point Energies = -956.416300

O	2.55114800	1.41538900	-0.36220600
O	2.54847700	-0.82796700	-0.22404000
O	5.23264800	-1.49228200	-0.51788500
H	5.27468100	-1.52786200	0.44935000
H	4.28029200	-1.28062900	-0.63062600
H	5.42242800	0.58838900	-0.15885600
O	5.15862400	1.39346700	0.31084700
H	4.19401300	1.46234000	0.07614600
O	4.20147000	-0.67001500	2.09582700
H	4.58555600	0.17086500	1.79319300
H	3.48005700	-0.78348000	1.44390200
C	2.02628400	0.28508700	-0.53439000
C	0.62700700	0.28045800	-1.14102400
C	-0.09672400	-1.03693500	-1.46726800
C	-0.56702200	0.65623700	-0.20055700
H	0.62425800	0.96830900	-1.99716000
C	-1.41760200	-0.39904700	-0.97513800
H	0.25477700	-1.82990400	-0.79622000
H	-0.05503000	-1.40110600	-2.50239800
H	-1.91858300	0.12453300	-1.80068000
C	-1.04015500	2.09799800	-0.26972100
H	-1.97074200	2.21587500	0.29936400
H	-0.26049800	2.76693900	0.12316000
H	-1.24933500	2.37869000	-1.31134500
C	-0.29275600	0.25256500	1.24370000
H	0.09609200	-0.77118500	1.31212700
H	0.46095500	0.92354100	1.67812200
H	-1.21604300	0.31967400	1.83540800
C	-2.43174900	-1.27502400	-0.26491600
H	-2.00390000	-1.71390200	0.64772300
H	-2.68666700	-2.13069300	-0.91086000
C	-3.76948200	-0.60176900	0.11965100
O	-3.93951300	0.59640000	-0.22483000
O	-4.58628800	-1.33667200	0.74029300
O	-6.60894200	0.57732100	0.70678200
H	-5.83039000	0.99395500	0.29449800
H	-6.16970200	-0.27689800	0.89481900

Cluster: *cis*-$PA^{2-}(H_2O)_4$

Isomer: iso C

Sum of electronic and zero-point Energies = -956.416286

O	2.44563000	-0.02960400	1.04855700
O	3.14475100	-0.08674100	-1.08458600
O	5.76964800	0.79775300	-0.97802200

H	6.02985600	-0.13512900	-1.00139900
H	4.79425500	0.69470200	-1.04010300
H	5.42501600	0.35901300	1.06774500
O	5.05611100	-0.20259900	1.76552200
H	4.08415600	-0.16418500	1.56826200
O	5.12607300	-2.01652600	-0.48920300
H	5.19898800	-1.70573200	0.42913200
H	4.34507100	-1.50416400	-0.78704700
C	2.26163900	0.07833100	-0.18492600
C	0.86800500	0.48214900	-0.69343300
H	0.99116600	1.49442500	-1.11374400
H	0.62614000	-0.16695300	-1.54598600
C	-0.24807000	0.48214200	0.33432700
C	-1.00883700	-0.81778200	0.68611000
C	-1.61840800	1.13610000	-0.01545300
H	0.13005100	0.93278500	1.26166300
C	-2.29135600	0.02325000	0.84626200
H	-0.65210700	-1.38880600	1.55004400
H	-1.10899300	-1.49114200	-0.17395000
H	-2.40069800	0.39415500	1.87489600
C	-3.66062900	-0.47157100	0.36254700
O	-3.72765200	-1.60589200	-0.17330200
O	-4.60709700	0.35296900	0.52382900
C	-1.99263300	0.98996200	-1.48809100
H	-3.04395700	1.27519700	-1.62863800
H	-1.35801200	1.63080800	-2.11763800
H	-1.88552900	-0.04830700	-1.82453700
C	-1.83275700	2.56902300	0.44324600
H	-1.22683900	3.26807400	-0.15560600
H	-2.89383900	2.83673700	0.34019900
H	-1.54654200	2.68170400	1.49811100
O	-6.52512600	-1.38197400	-0.51741500
H	-5.67040900	-1.84471200	-0.58943100
H	-6.15822600	-0.56719100	-0.11853800

Cluster: *cis*-$PA^{2-}(H_2O)_4$

Isomer: iso D

Sum of electronic and zero-point Energies = -956.405967

O	1.74561400	-0.13793500	0.82952600
O	2.25982900	0.02195200	-1.34669800
O	4.47378400	-1.65496400	-0.95696000
O	3.95664600	-1.51069400	1.87773800
H	3.62448700	-1.19127500	-1.12777000
H	4.44668300	-1.77766000	0.00735900

H	3.07484500	-1.24556500	1.54102300
H	4.37959500	-0.63884200	1.93350400
O	4.84290900	1.12457700	-1.42557100
H	5.11915500	0.19975300	-1.30239500
H	3.87883400	0.98915000	-1.51834600
O	4.14045700	1.32476600	1.38065000
H	3.25044300	0.94661200	1.23653000
H	4.49848300	1.37344300	0.47707700
C	1.45517300	0.10431900	-0.37347700
C	0.04009600	0.60111500	-0.69793500
H	0.12615400	1.70114600	-0.74092800
H	-0.20622700	0.27180000	-1.71491800
C	-1.04875200	0.21846600	0.28943900
C	-2.45968000	0.86792100	0.16785800
C	-1.72995400	-1.16847700	0.21762800
H	-0.67149500	0.38408600	1.30711600
C	-3.05706500	-0.49721900	0.62812000
H	-1.81103900	-1.54719100	-0.80888900
H	-1.32661000	-1.95872100	0.86128800
H	-3.17457700	-0.47940000	1.72131700
C	-2.85611400	1.17765800	-1.27357200
H	-3.92575100	1.42411400	-1.30703800
H	-2.27396900	2.02499000	-1.66729400
H	-2.69948400	0.30856500	-1.92451400
C	-2.74706200	2.06466000	1.05947700
H	-2.20125400	2.95840000	0.71473700
H	-3.82576300	2.27558300	1.04932300
H	-2.44435200	1.85459400	2.09483000
C	-4.40891000	-0.89211500	-0.00592200
O	-4.40635600	-1.81875600	-0.85054600
O	-5.38345300	-0.19038900	0.37914900

Cluster: *cis*-$PA^{2-}(H_2O)_4$

Isomer: iso E

Sum of electronic and zero-point Energies = -956.405613

O	1.45849400	-1.19244300	-0.08275000
O	1.97397700	0.88556000	-0.75918300
O	4.55193400	0.01952600	-1.50292600
O	3.95563800	-2.47513900	-0.18906200
H	3.62362500	0.31052700	-1.37819000
H	4.52840600	-0.88624300	-1.14806400
H	3.03744900	-2.16917900	-0.34043900
H	4.10656200	-2.09604100	0.69268800
O	4.14527600	1.69165900	0.80038800

H	4.68467700	1.22496600	0.14091200
H	3.26208800	1.58202300	0.39127400
O	3.32807000	-0.79364500	2.04382800
H	2.57614900	-0.90194300	1.42712700
H	3.68605000	0.07460900	1.79039500
C	1.16212000	-0.07352000	-0.58179300
C	-0.28284600	0.20756600	-0.96386900
C	-1.08965100	1.10382000	0.03091400
C	-1.39571100	-0.85129600	-0.84464600
H	-0.28874700	0.69063300	-1.95002600
C	-2.34680300	0.26432200	-0.35197900
H	-1.68665700	-1.39545700	-1.74926000
H	-1.15511800	-1.56955200	-0.05171000
H	-2.82516100	0.72534900	-1.22648200
C	-1.13426900	2.58950800	-0.28531900
H	-1.83497900	3.10583000	0.38950100
H	-0.13690200	3.03741900	-0.16930700
H	-1.47163000	2.75134600	-1.31800500
C	-0.63566500	0.87993800	1.47082200
H	0.35103900	1.33729500	1.63319300
H	-1.35256100	1.32925900	2.17207600
H	-0.55124200	-0.18810200	1.70402800
C	-3.42669300	-0.02936000	0.67006400
H	-3.71621900	0.90651800	1.17948600
H	-3.06360400	-0.70856900	1.45367900
C	-4.75256400	-0.62173400	0.09313000
O	-4.94878400	-0.48133000	-1.13855400
O	-5.50969800	-1.15120800	0.94490600

Cluster: *cis*-$PA^{2-}(CH_3CN)$

Isomer: iso A

Sum of electronic and zero-point Energies = -783.454731

C	2.13083300	0.84183800	-0.14838100
C	2.63762100	-0.53349900	-0.68068300
C	1.28360000	-1.14390900	-0.26125400
C	0.68071900	0.28122800	-0.26357000
C	2.47017800	2.05953900	-0.99339500
C	2.57435100	1.06635500	1.29519500
C	3.98507500	-1.03547300	-0.11862300
C	-0.37739800	0.68573500	0.74709500
C	-1.84040100	0.31045500	0.39692600
O	3.96498600	-2.02204500	0.65560700
O	4.98448200	-0.35812000	-0.48679900
O	-2.11390700	0.04743700	-0.80008500

O	-2.65459800	0.34406400	1.36479500
H	1.36456900	-1.56671600	0.74804700
H	0.82041400	-1.88432000	-0.92398800
H	2.37979700	0.17970700	1.91134900
H	3.65650400	1.25396000	1.31744900
H	2.04470200	1.92378800	1.73777100
H	1.98450100	2.96591000	-0.59482000
H	3.55952300	2.20853400	-1.00131600
H	2.13074400	1.91441100	-2.02867300
H	0.29676800	0.50129500	-1.26903600
H	2.72139400	-0.47249800	-1.77604100
H	-0.15456700	0.27745600	1.74226000
H	-0.37642100	1.78438600	0.86020100
C	-4.98153300	-0.30095200	-0.47064300
H	-4.75934400	0.47504200	-1.20930900
H	-4.40470800	-0.05171800	0.44033700
H	-4.58638600	-1.24779100	-0.85089300
C	-6.42238400	-0.39944700	-0.24475300
N	-7.56702200	-0.47762200	-0.07413700

Cluster: *cis*-$PA^{2-}(CH_3CN)$

Isomer: iso B

Sum of electronic and zero-point Energies = -783.453760

C	-0.79893400	1.07515800	0.13856000
C	0.02505400	0.26414900	-0.90995800
C	-1.07765300	-0.81345600	-0.87568700
C	-2.04603100	0.24518200	-0.29583800
C	-0.86991800	2.57919000	-0.07131000
C	-0.33727300	0.76292300	1.55956900
C	1.48534100	-0.04271800	-0.54698600
C	-3.10899900	-0.13968900	0.71612100
C	-4.44130800	-0.70305500	0.12829900
O	1.78618200	-1.21322100	-0.20654900
O	2.26779300	0.95407300	-0.59583300
O	-4.69764000	-0.43050000	-1.06982000
O	-5.15121900	-1.34782900	0.94308400
H	-0.82041500	-1.58979700	-0.14435900
H	-1.36471500	-1.29044800	-1.81981800
H	-0.23774500	-0.31822000	1.71489700
H	0.64814000	1.21756100	1.73438600
H	-1.05441600	1.15663800	2.29472100
H	-1.57390400	3.03867400	0.64154300
H	0.12456800	3.02737500	0.06775200
H	-1.21591800	2.80699300	-1.08910300

H	-2.54293400	0.76179200	-1.12815800
H	0.01510600	0.81534100	-1.86110300
H	-2.72334900	-0.86884300	1.44201500
H	-3.39932600	0.75319900	1.29824400
C	4.64336100	-0.79133000	0.14125800
H	4.24411900	-1.16649400	1.08836000
H	4.04213300	0.09518900	-0.13524900
H	4.46103400	-1.55206700	-0.62368800
C	6.07392800	-0.51469800	0.26014200
N	7.21018200	-0.30243000	0.35535500

Cluster: *cis*-$PA^{2-}(CH_3CN)_2$

Isomer: iso A

Sum of electronic and zero-point Energies = -916.155234

C	0.65340300	1.40972400	0.04728400
C	1.36373200	0.35778600	-0.86011100
C	0.18366800	-0.59989400	-0.59784700
C	-0.67100800	0.62508500	-0.19507300
C	0.69675700	2.85276900	-0.42862900
C	1.15011300	1.31608200	1.48782300
C	2.81166000	0.00510800	-0.48868900
C	-1.71513600	0.52348900	0.90145200
C	-3.10187500	-0.01893000	0.46710400
O	3.03580700	-1.12226400	0.02514300
O	3.65712500	0.91689000	-0.71023000
O	-3.38865900	0.00892100	-0.75498100
O	-3.84821800	-0.41050800	1.40900500
H	0.41373900	-1.24894900	0.25586000
H	-0.17968900	-1.21441900	-1.42916100
H	1.17212400	0.27572900	1.83463200
H	2.17455700	1.70856300	1.54926400
H	0.50046900	1.89550100	2.16012300
H	0.07136100	3.49596300	0.21152900
H	1.73224000	3.22136400	-0.40481300
H	0.32407600	2.92855900	-1.45948500
H	-1.15685900	1.02686100	-1.09429200
H	1.35447000	0.72739300	-1.89542300
H	-1.35895800	-0.09205400	1.73860700
H	-1.90885500	1.52728000	1.31901900
C	6.05173300	-0.59471500	-0.11204000
H	6.03830200	0.30792500	0.50559600
H	6.02910000	-0.28104300	-1.15992700
H	5.10853900	-1.13407400	0.08402900
C	7.24828400	-1.38880500	0.16348500

N	8.20370700	-2.00916800	0.38016100
C	-6.20079900	-0.71030500	-0.49637000
H	-5.59404100	-0.70856800	0.42849100
C	-7.61037300	-1.02316800	-0.26836300
N	-8.73008100	-1.26894000	-0.09305300
H	-6.09496600	0.28029500	-0.94877300
H	-5.75038300	-1.43923800	-1.17668600

Cluster: *cis*-$PA^{2-}(CH_3CN)_2$

Isomer: iso B

Sum of electronic and zero-point Energies = -916.146704

C	0.93759200	0.70691900	0.02215800
C	2.45597900	0.41075900	0.21758700
C	2.06840800	-0.63334600	1.29110000
C	0.69754700	0.06012100	1.42269900
C	0.30476400	-0.13084400	-1.08615300
C	0.53901300	2.16591300	-0.12958400
C	-0.60114800	-0.73587400	1.58108100
O	-0.54712200	-1.98457500	1.62228500
O	-1.66374600	-0.03365400	1.60362900
H	2.70509600	-0.69214800	2.18050200
H	1.94297300	-1.63891200	0.87078500
H	1.00597500	2.77361200	0.65699800
H	0.86423900	2.55939000	-1.10582300
H	-0.55202400	2.27638600	-0.04653000
H	-0.78977200	-0.02615500	-1.05080200
H	0.66351000	0.19577600	-2.07217100
H	0.54621800	-1.19415900	-0.96402600
H	2.92408400	1.27088000	0.71470200
C	-2.81840600	-2.30959800	-0.13582500
H	-2.76410100	-1.43096500	0.52866200
H	-2.77155400	-3.20156000	0.49459900
H	-1.92839400	-2.28921100	-0.77303700
C	-4.03159300	-2.31399300	-0.95086900
N	-4.99514400	-2.30854500	-1.59521300
C	-3.36105300	1.32499600	-0.53381200
H	-2.67153500	1.57522000	-1.34796700
C	-4.21223700	2.48003900	-0.25647800
N	-4.89287100	3.39403200	-0.05077500
H	-3.98990600	0.48241100	-0.84515700
H	-2.76985700	1.03014600	0.35291900
H	0.71736000	0.85284200	2.18370600
C	3.32693500	0.02162600	-0.96166100
H	3.03858100	-0.95921300	-1.36516800

H	3.18542600	0.74987000	-1.77986400
C	4.86403900	-0.00377900	-0.68409500
O	5.27297700	0.64921300	0.30661300
O	5.54298200	-0.65476500	-1.51844000

Cluster: *cis*-$PA^{2-}(CH_3OH)$

Isomer: iso A

Sum of electronic and zero-point Energies = -766.420461

C	1.76542600	0.85676300	-0.11524900
C	2.34240800	-0.48312600	-0.66575000
C	0.98629000	-1.14608600	-0.34511500
C	0.34215300	0.26092700	-0.33593500
C	2.11703300	2.11395800	-0.89448400
C	2.11709600	1.03694800	1.35944500
C	3.67146000	-0.96497600	-0.04500000
C	-0.78558000	0.60191000	0.62223300
C	-2.21234500	0.22808200	0.15572100
O	3.63751600	-1.97216500	0.70148500
O	4.66947100	-0.25084700	-0.34018400
O	-2.41174400	0.01251100	-1.05628700
O	-3.08535400	0.21655900	1.08184000
H	1.02308600	-1.59939400	0.65360000
H	0.58354900	-1.87672400	-1.05615100
H	1.91141300	0.12241500	1.92932500
H	3.19079800	1.24996400	1.45388500
H	1.53978200	1.86347700	1.80111100
H	1.58538900	2.99202600	-0.49141800
H	3.20073100	2.29021900	-0.83594300
H	1.83939300	1.99943800	-1.95177600
H	0.01308400	0.50661500	-1.35476100
H	2.48467300	-0.37957400	-1.75179900
H	-0.62234000	0.14824500	1.60911000
H	-0.81059900	1.69326700	0.78830500
O	-5.61955500	-0.11242300	0.54526300
H	-4.64552800	0.02777800	0.76653900
C	-5.64750700	-0.74313400	-0.70920700
H	-4.67551500	-0.64830500	-1.21788500
H	-5.88999400	-1.82078700	-0.61569000
H	-6.42919200	-0.28534000	-1.34334300

Cluster: *cis*-$PA^{2-}(CH_3OH)$

Isomer: iso B

Sum of electronic and zero-point Energies = -766.420317

C	-0.37403500	0.98367100	0.14118300

C	0.39162500	0.10655700	-0.89793600
C	-0.79364000	-0.87888100	-0.87381200
C	-1.67937500	0.25713100	-0.30783200
C	-0.31617700	2.48796900	-0.06934300
C	0.04362800	0.63422900	1.56714000
C	1.81646200	-0.31728400	-0.52576300
C	-2.78058100	-0.03715300	0.69368200
C	-4.14687400	-0.49965400	0.09602400
O	2.03801400	-1.50284400	-0.20978400
O	2.66439700	0.63579600	-0.54855800
O	-4.36679100	-0.22535300	-1.10893200
O	-4.91592200	-1.07228500	0.91107500
H	-0.61023900	-1.67167100	-0.13783300
H	-1.10712000	-1.33350300	-1.82037500
H	0.04939000	-0.45131800	1.72233700
H	1.06079600	1.00524000	1.75537800
H	-0.64777700	1.08528100	2.29400900
H	-0.99243600	3.00523300	0.63068700
H	0.70964000	2.85090400	0.08936000
H	-0.62203000	2.74364200	-1.09331000
H	-2.12273400	0.81004400	-1.14726600
H	0.43385000	0.65427200	-1.85019800
H	-2.45966700	-0.78862000	1.42849200
H	-3.00689500	0.87953300	1.26717000
O	5.19640200	0.19533900	-0.09692200
C	5.23714900	-0.98236200	0.66629300
H	5.42846300	-0.76636900	1.73669300
H	4.28814200	-1.53530200	0.58735200
H	6.05865800	-1.63191200	0.31200700
H	4.22206500	0.37397500	-0.28735800

Cluster: *cis*-$PA^{2-}(CH_3OH)_2$

Isomer: iso A

Sum of electronic and zero-point Energies = -882.087310

C	0.72057100	1.16967600	-0.03506500
C	1.37871400	0.01131300	-0.84754000
C	0.10306000	-0.82154900	-0.61193000
C	-0.65524600	0.49443000	-0.31918100
C	0.92150500	2.57458500	-0.57940400
C	1.12574800	1.10992800	1.43535000
C	2.75767600	-0.46175200	-0.37492300
C	-1.76192500	0.54545500	0.71718200
C	-3.16333300	0.11009900	0.22583300
O	2.85593400	-1.56054800	0.20598000

O	3.69693500	0.36766300	-0.60715800
O	-3.36684300	0.02013100	-1.00100800
O	-4.00922100	-0.08661400	1.15444700
H	0.22290900	-1.44466600	0.28308900
H	-0.26950900	-1.44177500	-1.43454800
H	1.03414500	0.09199100	1.83326900
H	2.17617500	1.41448200	1.54049800
H	0.49423300	1.77825500	2.03881300
H	0.32772600	3.30545500	-0.00684600
H	1.98380900	2.85084100	-0.51880200
H	0.60787600	2.62580300	-1.63119400
H	-1.05211000	0.88863600	-1.26426700
H	1.46159300	0.32580000	-1.89751100
H	-1.51057700	-0.05746600	1.60042600
H	-1.88374900	1.58059800	1.07998900
O	6.20380100	-0.16240300	-0.07015700
H	5.24410100	0.05663500	-0.27528100
C	6.19852900	-1.42248700	0.55120800
H	6.63703600	-1.36001600	1.56563700
H	5.17353200	-1.81571600	0.63460800
H	6.80785800	-2.14456100	-0.02569500
C	-6.49861900	-1.12740000	-0.69552300
H	-5.56093600	-0.89679700	-1.22486700
H	-7.34992000	-0.76441900	-1.29916400
H	-6.59490000	-2.22921000	-0.62024600
O	-6.52379800	-0.51846900	0.56974300
H	-5.56383000	-0.33574300	0.81127700

Cluster: *cis*-$PA^{2-}(CH_3OH)_2$

Isomer: iso B

Sum of electronic and zero-point Energies = -882.079457

C	0.92530800	-0.70270600	0.72803400
C	0.20768400	-0.81046100	-0.65490100
C	1.40432900	-0.06974500	-1.28414000
C	2.25378000	-0.47967800	-0.05728500
C	0.85226900	-1.92920900	1.62275300
C	0.46738400	0.53647300	1.49287000
C	-1.21806700	-0.26733000	-0.70988500
C	3.33100800	0.43827400	0.48785900
C	4.72156600	0.34798600	-0.21778500
O	-1.41611500	0.84336600	-1.26605300
O	-2.08808500	-0.97853500	-0.12769300
O	4.94823100	-0.67774000	-0.90455100
O	5.49510600	1.31250900	0.01285500

H	1.20890900	1.00904600	-1.31341500
H	1.75400200	-0.40074500	-2.26805300
H	0.46460900	1.42477100	0.85003900
H	-0.55609800	0.38883500	1.86570700
H	1.13394400	0.72863500	2.34570400
H	1.49265300	-1.80020000	2.51004300
H	-0.18348300	-2.09697600	1.95155500
H	1.19447900	-2.82069900	1.07953500
H	2.71292300	-1.45678000	-0.25966700
H	0.18613800	-1.86682000	-0.95551400
H	3.00947500	1.48898800	0.47000300
H	3.52189500	0.19124300	1.54722100
O	-4.64203000	-1.66841900	-0.52392500
H	-3.68283800	-1.43711500	-0.45022300
C	-5.34845400	-0.57219100	0.00168100
H	-5.28650100	-0.53208200	1.10570100
H	-4.97773600	0.38706700	-0.39120700
H	-6.40989100	-0.68217000	-0.27129300
C	-3.26187600	2.01020800	0.99126200
H	-4.18035000	2.29011000	1.53149200
H	-2.42263900	2.58946800	1.41779200
H	-3.06232700	0.94076400	1.16378500
O	-3.44454600	2.28182100	-0.37721700
H	-2.74724500	1.74091100	-0.83931200

Cluster: *cis*-$PA^{2-}(CH_3CN)(H_2O)$

Isomer: iso A

Sum of electronic and zero-point Energies = -859.874128

C	-0.19938000	1.24955300	0.02311500
C	0.59233800	0.20974100	-0.82977000
C	-0.56164900	-0.78798600	-0.60424500
C	-1.48040700	0.40892700	-0.26327100
C	-0.18988400	2.68383400	-0.47993000
C	0.23127800	1.20204800	1.48696000
C	2.03092900	-0.08712100	-0.38228400
C	-2.56518500	0.28580100	0.79084600
C	-3.91144400	-0.31468200	0.31423200
O	2.27067800	-1.18720100	0.17260400
O	2.85674000	0.85065700	-0.59411600
O	-4.15488100	-0.30259000	-0.91936800
O	-4.67317700	-0.73001200	1.23188500
H	-0.34602900	-1.41362300	0.27052800
H	-0.86251600	-1.42916400	-1.44029900
H	0.27904300	0.16961100	1.85435000

H	1.23441900	1.63835600	1.59020800
H	-0.47301800	1.76542300	2.11675600
H	-0.86956900	3.31333900	0.11708900
H	0.82784600	3.09473600	-0.41489900
H	-0.51539400	2.72518400	-1.52850000
H	-1.94175600	0.77624200	-1.18957000
H	0.61930100	0.56064300	-1.87109500
H	-2.22121000	-0.30086800	1.65326100
H	-2.81474900	1.28872100	1.17973100
C	5.17575200	-0.95535700	0.20182100
H	4.61100300	-0.07067300	-0.14625700
H	4.84889100	-1.80354600	-0.40723800
H	4.87085300	-1.14749600	1.23497300
C	6.62597500	-0.79130400	0.11806400
N	7.77747200	-0.66945200	0.05362400
O	-6.78043400	-1.25121400	-0.50723900
H	-6.03651900	-0.94558700	-1.05861300
H	-6.29424900	-1.19297600	0.34084900

Cluster: *cis*-$PA^{2-}(CH_3CN)(H_2O)$

Isomer: iso B

Sum of electronic and zero-point Energies = -859.873945

C	1.54233700	1.12452600	-0.10110400
C	2.11602800	-0.13417500	-0.82410900
C	0.82166700	-0.88394500	-0.44980800
C	0.12904900	0.48538200	-0.25691600
C	1.77356300	2.46099700	-0.78730600
C	2.01483400	1.18716400	1.34924500
C	3.50171300	-0.60885300	-0.36845600
C	-0.92386200	0.68613800	0.81677500
C	-2.36330200	0.24052100	0.44971300
O	3.57387100	-1.64071000	0.34537700
O	4.46317300	0.12786700	-0.73811300
O	-2.62038400	0.00737900	-0.75678200
O	-3.17309700	0.18456800	1.41894100
H	0.96133400	-1.41892300	0.49766300
H	0.38589100	-1.56651600	-1.18768000
H	1.90084600	0.21667300	1.84728800
H	3.08121300	1.45016500	1.37862400
H	1.44193800	1.93934600	1.91155200
H	1.23244600	3.26785600	-0.26699000
H	2.84737900	2.69670700	-0.79297600
H	1.42022000	2.42468900	-1.82707400
H	-0.29563700	0.80264200	-1.21899500

H	2.15964600	0.07258700	-1.90273200
H	-0.64356800	0.17753300	1.74950100
H	-0.99923200	1.75903700	1.06584900
C	-5.46911200	-0.51510700	-0.45182900
H	-5.26351600	0.27641400	-1.17857500
H	-4.90950700	-0.26022400	0.46752000
H	-5.04421900	-1.44553100	-0.84067100
C	-6.90814200	-0.66021900	-0.23969100
N	-8.05113400	-0.77534300	-0.08010100
O	6.39628600	-1.50461100	0.41571900
H	6.01869500	-0.74922000	-0.08035800
H	5.53658600	-1.90635000	0.63854700

Cluster: *cis*-$PA^{2-}(CH_3CN)(H_2O)$

Isomer: iso C

Sum of electronic and zero-point Energies = -859.871155

O	5.49945900	-0.22012700	-1.06259500
O	4.58286700	-0.20352700	1.00255900
H	-2.87572000	1.77336800	-1.49153600
O	-3.32305300	2.45179100	-0.95496900
H	-2.91382400	2.18729400	-0.10226700
C	4.56037800	-0.37807600	-0.24136100
C	0.67349500	-1.46251600	-0.46299800
C	1.29604200	0.33302700	0.57485500
C	-0.04395600	-0.47072500	0.47004900
H	0.44237600	-2.53101100	-0.35105000
H	0.51003000	-1.16999100	-1.50754700
H	-0.25637200	-0.91704700	1.45141800
C	1.35012400	1.47086800	-0.43824200
H	0.66711500	2.27437600	-0.12861200
H	2.37290100	1.86756100	-0.49999700
H	1.03844900	1.13837300	-1.43632500
C	1.66858300	0.83794300	1.95841900
H	1.62395000	0.01574500	2.68667400
H	2.69837800	1.21668800	1.94989500
H	0.96449400	1.62262400	2.27406800
C	-1.28698200	0.28984400	0.00858200
O	-1.84714100	1.01554600	0.88482100
O	-1.65993200	0.16558000	-1.18963800
C	-4.47693500	-0.35230700	0.05083800
H	-4.72039000	0.65069300	-0.31838500
H	-3.75348500	-0.78810900	-0.64871100
H	-3.97331500	-0.23831300	1.01707400
C	-5.67766300	-1.17582900	0.16958400

N	-6.63513900	-1.82274400	0.26224700
C	2.03064000	-0.95275300	0.08025300
H	2.32356600	-1.52485900	0.97134700
C	3.21882600	-0.87099700	-0.85993900
H	3.41398100	-1.87258700	-1.27900900
H	2.99092400	-0.23056400	-1.72443100

Cluster: *cis*-$PA^{2-}(CH_3CN)(H_2O)$

Isomer: iso D

Sum of electronic and zero-point Energies = -859.854451

C	-1.49883300	1.06334400	0.10905600
C	-0.70943900	0.17631400	-0.90436800
C	-1.85888800	-0.84871800	-0.83417900
C	-2.78035000	0.27310500	-0.29918200
C	-1.50126100	2.55942300	-0.16034600
C	-1.05658500	0.78576800	1.54335500
C	0.73284100	-0.18161300	-0.52407400
C	-3.86098800	-0.02796500	0.72225400
C	-5.21133000	-0.56228300	0.14846000
O	0.98361800	-1.34983500	-0.13931700
O	1.56128800	0.77721300	-0.60602300
O	-5.45718200	-0.31264100	-1.05687400
O	-5.94278800	-1.16005700	0.97944700
H	-1.64048200	-1.60779400	-0.07269900
H	-2.16376400	-1.34768700	-1.76109000
H	-1.00178500	-0.29196100	1.73910800
H	-0.05518200	1.20782700	1.70890100
H	-1.76138900	1.23401300	2.25886200
H	-2.18483200	3.07877500	0.53092600
H	-0.48799900	2.96796900	-0.03552000
H	-1.83480500	2.76180600	-1.18757800
H	-3.25286900	0.77907400	-1.15200300
H	-0.69180900	0.69096000	-1.87569500
H	-3.50681600	-0.74172600	1.47873400
H	-4.11911700	0.89877700	1.26544200
C	3.83307400	-1.01923800	0.12414900
H	3.22447100	-0.13385300	-0.15895000
H	3.62290900	-1.79991700	-0.61315400
H	3.46959800	-1.36277000	1.09718700
C	5.26301900	-0.74242200	0.18043100
N	6.39910500	-0.52039300	0.22168000
O	9.14110300	0.43605100	0.14371900
H	8.93039300	1.31386400	-0.18561600
H	8.26387800	0.01525900	0.21042600

Cluster: *cis*-$PA^{2-}(CH_3CN)(H_2O)_2$

Isomer: iso A

Sum of electronic and zero-point Energies = -936.290306

O	4.95545400	-0.08001700	-1.26791900
O	4.09722700	-0.41239600	0.79076600
H	-3.39576600	1.89173300	-1.29008200
O	-3.84565100	2.54397600	-0.72095600
H	-3.44327000	2.23804800	0.11675300
C	4.02487800	-0.36656900	-0.46400800
C	0.14153800	-1.37349200	-0.77924700
C	0.77997200	0.22514000	0.53732500
C	-0.56319000	-0.54647200	0.30984100
H	-0.08911600	-2.44573000	-0.84005800
H	-0.03336000	-0.91618500	-1.76079300
H	-0.77656800	-1.14733300	1.20469000
C	0.82774100	1.51844300	-0.26841100
H	0.15020400	2.25814000	0.17944900
H	1.85021900	1.92098800	-0.27432200
H	0.50409400	1.35892100	-1.30489800
C	1.16386000	0.48555700	1.98389700
H	1.13704300	-0.45053600	2.55893800
H	2.18610800	0.88092600	2.03831300
H	0.45286800	1.19298300	2.43519500
C	-1.80456600	0.28428600	-0.01700600
O	-2.31783300	0.91257900	0.95573000
O	-2.21863900	0.30084100	-1.20788900
C	-5.00909300	-0.33962300	-0.02147100
H	-5.30098400	0.66288500	-0.35337400
H	-4.39221400	-0.79024900	-0.80665600
H	-4.37147600	-0.21658100	0.86275900
C	-6.18355800	-1.15840100	0.26882700
N	-7.12038700	-1.80161700	0.49670300
C	1.50478000	-0.95942500	-0.17685100
H	1.81419000	-1.67398300	0.59806300
C	2.66946400	-0.71812300	-1.11862300
H	2.84065600	-1.62583800	-1.72033000
H	2.43164200	0.07389300	-1.84278000
O	6.88330800	0.11410300	0.72270300
H	6.04881800	-0.06732700	1.19076500
H	6.48772900	0.12594900	-0.17366000

Cluster: *cis*-$PA^{2-}(CH_3CN)(H_2O)_2$

Isomer: iso B

Sum of electronic and zero-point Energies = -936.289504

O	2.62436200	0.81621100	-1.56833000
O	2.12031300	0.80815900	0.62373100
H	-6.11758600	-0.67424300	-0.96516900
O	-6.82599500	-0.13853800	-0.56235700
H	-6.25997000	0.25702300	0.13069000
C	1.92307500	0.47079300	-0.57339700
C	-1.42986700	-1.66869400	0.01124000
C	-1.36404400	0.45337300	0.43538100
C	-2.38128100	-0.69647700	0.73208400
H	-1.30216600	-2.67421300	0.43404300
H	-1.72838100	-1.75916000	-1.04051000
H	-2.39877200	-0.87684900	1.81600200
C	-1.72435900	1.19743700	-0.84621300
H	-2.61376900	1.81731600	-0.67012000
H	-0.89136100	1.84059900	-1.16464400
H	-1.96539000	0.50152200	-1.65959500
C	-1.11270600	1.43577400	1.56701400
H	-0.82244700	0.89847900	2.48046500
H	-0.29455300	2.12142100	1.30838400
H	-2.03105500	2.00437400	1.77265700
C	-3.82590900	-0.50251400	0.25099100
O	-4.50872600	0.32246200	0.92211100
O	-4.19998100	-1.14632200	-0.76365800
C	4.88791400	-0.52911800	0.08565000
H	5.25032800	0.50342500	0.15248100
H	4.09074000	-0.64936100	0.82783800
H	4.44313600	-0.65613500	-0.90778200
C	5.97113900	-1.48347400	0.30929700
N	6.83463500	-2.23559300	0.48717400
C	-0.28381500	-0.65067700	0.21309100
H	0.21654300	-0.82549400	1.17479600
C	0.77043100	-0.50721000	-0.86885200
H	1.24444200	-1.48991600	-1.03661600
H	0.32141400	-0.22526100	-1.83028200
O	4.17431100	2.59784800	-0.12232200
H	3.55801900	2.21939500	0.53070200
H	3.80063600	2.12239700	-0.89467100

Cluster: *cis*-$PA^{2-}(CH_3CN)(H_2O)_2$

Isomer: iso C

Sum of electronic and zero-point Energies = -936.285842

O	3.36244700	0.76809700	-0.78120400
O	2.72545100	-1.20743200	0.10120400

O	-5.95668500	-1.75676300	-0.84834400
H	-5.75762600	-1.87739900	0.09087300
H	-5.14273400	-1.24422900	-1.09189400
H	-5.85792300	0.18339500	1.19498100
O	-6.78891500	0.40282300	0.97986000
H	-6.88699400	-0.09547500	0.15620000
C	2.51504200	-0.13570200	-0.51730500
C	1.08311700	0.17230800	-0.97892100
C	-0.09139000	-0.78844600	-0.70443900
C	0.31976100	1.26698900	-0.16953400
H	1.11493500	0.47581500	-2.03477100
C	-0.98038300	0.44191100	-0.40868200
H	0.11668300	-1.38128000	0.19468000
H	-0.41437100	-1.45725300	-1.50979300
H	-1.44295300	0.77940900	-1.34561700
C	0.35544300	2.67610200	-0.73794200
H	-0.30785300	3.34635800	-0.16759000
H	1.38167300	3.06792700	-0.69596600
H	0.02634400	2.67681200	-1.78617100
C	0.76066300	1.27697800	1.29198300
H	0.78789400	0.26194200	1.70680400
H	1.77515500	1.69210200	1.36585300
H	0.07699400	1.88706200	1.90039000
C	-2.05140800	0.38755700	0.66468200
H	-2.30387600	1.41104200	0.99086900
H	-1.69337500	-0.13774100	1.56018200
C	-3.39136700	-0.25320700	0.25236700
O	-3.63021300	-0.39065200	-0.97481300
O	-4.16895200	-0.56456300	1.20060600
C	5.60693400	-0.94250100	0.38645800
H	5.35095100	-1.84085800	-0.18310800
H	5.09138100	-0.09494400	-0.10002300
H	5.17806000	-1.04844900	1.38731800
C	7.05735200	-0.77645300	0.46349700
N	8.20857000	-0.65278900	0.52790600

Cluster: *cis*-$PA^{2-}(CH_3CN)(H_2O)_2$

Isomer: iso D

Sum of electronic and zero-point Energies = -936.279700

C	1.12289200	0.14520700	1.06009200
C	0.50479100	-1.15688400	0.45929000
C	1.62817700	-1.15246900	-0.59545500
C	2.45343300	-0.24456600	0.34677700
C	1.16018000	0.24161300	2.57629500

C	0.47246300	1.39228100	0.46778000
C	-0.96995800	-1.10340200	0.07859100
C	3.37383000	0.82311700	-0.21075400
C	4.78833400	0.32822200	-0.65182600
O	-1.29096400	-0.99276000	-1.12585400
O	-1.77905100	-1.13777400	1.06430700
O	5.17126500	-0.77681900	-0.19640100
O	5.41669000	1.12036200	-1.39824000
H	1.29925700	-0.62439200	-1.49865200
H	2.07089000	-2.11263700	-0.88065900
H	0.39207300	1.31982200	-0.62379800
H	-0.53924400	1.51806700	0.87902900
H	1.06468400	2.28520200	0.71095500
H	1.74318700	1.12128400	2.89146800
H	0.14114800	0.32831800	2.98007000
H	1.63095000	-0.65304900	3.00579700
H	3.04244500	-0.88258400	1.01925100
H	0.63995000	-1.97058700	1.18451300
H	2.91401300	1.34233200	-1.06307200
H	3.55451900	1.59219000	0.56061100
C	-3.25584900	1.26931500	-0.54774100
H	-2.32842300	1.50873900	-1.07773900
H	-2.99164700	0.75677400	0.38512500
H	-3.83937000	0.57516100	-1.16355500
C	-4.02062400	2.48631800	-0.28000700
N	-4.62882100	3.45121000	-0.07651300
O	-4.29463100	-1.70031900	0.86532800
H	-4.29475800	-2.59844400	1.20601000
H	-3.31234800	-1.44457800	0.89850000
O	-3.86974300	-1.66036900	-1.98652800
H	-2.93220700	-1.44893400	-1.78760300
H	-4.22791000	-1.76223700	-1.08980600

Cluster: *cis*-$PA^{2-}(CH_3OH)(H_2O)$

Isomer: iso A

Sum of electronic and zero-point Energies = -842.840005

C	0.21779600	1.08982700	0.08539900
C	0.92118800	0.05398400	-0.84658900
C	-0.30354900	-0.86643100	-0.67540800
C	-1.12568100	0.37037600	-0.24155900
C	0.33130400	2.54976400	-0.32207400
C	0.65676000	0.91028400	1.53614300
C	2.33102100	-0.38657800	-0.43704300
C	-2.20895400	0.25574800	0.81542500

C	-3.60032200	-0.20357400	0.31225300
O	2.49106300	-1.51625900	0.06554600
O	3.22710600	0.49913100	-0.62837900
O	-3.86442400	-0.03739000	-0.90637700
O	-4.37203600	-0.66818500	1.19679700
H	-0.13137000	-1.56658300	0.15116900
H	-0.65725900	-1.42324000	-1.55042400
H	0.62399500	-0.14465000	1.83408800
H	1.69305300	1.25676100	1.65231100
H	0.00666200	1.48589200	2.21135800
H	-0.29233200	3.18664100	0.32578900
H	1.37737800	2.87953000	-0.24778200
H	-0.00378300	2.68447000	-1.35976300
H	-1.56691600	0.83467400	-1.13370900
H	0.96962400	0.47248100	-1.86157900
H	-1.90513600	-0.41426800	1.63066700
H	-2.37724600	1.24602500	1.27388600
O	5.76278200	0.04371500	-0.16390700
C	5.81256800	-1.21539000	0.45726700
H	4.80653700	-1.65563100	0.53554300
H	6.45627600	-1.90737400	-0.11877800
H	6.24450700	-1.13505000	1.47348600
O	-6.54443100	-0.81750800	-0.53939500
H	-6.04479900	-0.89834400	0.29863600
H	-5.78395000	-0.50948400	-1.06698700
H	4.79147800	0.23205500	-0.34507600

Cluster: *cis*-$PA^{2-}(CH_3OH)(H_2O)$

Isomer: iso B

Sum of electronic and zero-point Energies = -842.839002

C	1.13257000	1.13648500	-0.05603100
C	1.69728600	-0.09879800	-0.82509300
C	0.42612900	-0.87421800	-0.42437500
C	-0.27713700	0.48140700	-0.17550100
C	1.32202500	2.48953400	-0.72212200
C	1.65499500	1.17544900	1.37771600
C	3.10274800	-0.56345300	-0.42222000
C	-1.28637800	0.64121300	0.94732900
C	-2.72821600	0.17042200	0.64101000
O	3.20968200	-1.60325700	0.27585800
O	4.04311300	0.18978800	-0.81204300
O	-3.09623800	0.21951000	-0.57188300
O	-3.42543400	-0.17419800	1.61948700
H	0.60523500	-1.42978700	0.50432100

H	-0.02369400	-1.54607800	-1.16399700
H	1.56249500	0.19577900	1.86186500
H	2.72047500	1.44343900	1.37465000
H	1.09828100	1.91448000	1.97298700
H	0.78453200	3.27757900	-0.17025000
H	2.39152700	2.74223600	-0.75519300
H	0.93772700	2.46784400	-1.75111100
H	-0.74470600	0.81933100	-1.10986400
H	1.70349900	0.13151200	-1.89959300
H	-0.95193100	0.13152300	1.86009600
H	-1.37758200	1.71272900	1.19958700
O	-5.61906300	-0.27584700	-1.11726300
C	-5.98815000	-1.26559100	-0.19221300
H	-7.05661700	-1.14788400	0.06153900
H	-5.85789700	-2.28492700	-0.60797200
H	-5.38902300	-1.18774300	0.72817200
O	6.02706100	-1.41199400	0.30296600
H	5.63085600	-0.66142600	-0.18548200
H	5.17677700	-1.82947700	0.53362800
H	-4.65815300	-0.05583700	-0.92134600

Cluster: *cis*-$PA^{2-}(CH_3OH)(H_2O)$

Isomer: iso C

Sum of electronic and zero-point Energies = -842.831054

C	0.90809700	1.08314600	0.43685700
C	-0.13183300	-0.07483000	0.54933100
C	0.93135100	-1.02911000	-0.03010000
C	2.01812900	-0.01175800	0.39216600
C	0.95508200	2.06487400	1.59611900
C	0.75629400	1.83297300	-0.88378000
C	-1.48457900	0.15200600	-0.12500400
C	3.26782900	0.18807900	-0.44387300
C	4.42765200	-0.82594200	-0.18862800
O	-1.75734800	-0.48265800	-1.17428700
O	-2.22898000	1.01324000	0.44205100
O	4.39683800	-1.46973100	0.88815100
O	5.30668900	-0.86233400	-1.08796600
H	0.82437100	-1.09794800	-1.11958700
H	1.00185200	-2.03883500	0.38867000
H	0.67032700	1.13759000	-1.72753000
H	-0.15558500	2.44586900	-0.86063700
H	1.62466400	2.48446800	-1.05909500
H	1.80167800	2.76113300	1.48276500
H	0.02055600	2.64292400	1.63794900

H	1.07723900	1.52960800	2.54777100
H	2.33101700	-0.24077400	1.41999800
H	-0.31199500	-0.27855200	1.61416400
H	3.03695700	0.17473100	-1.51823500
H	3.69515700	1.18449800	-0.23248600
O	-5.64431300	-1.09852300	0.17704900
C	-4.49971500	-1.58251800	0.85575700
H	-4.77643600	-2.51878800	1.36179500
H	-3.66743600	-1.77848300	0.16249600
H	-4.13458500	-0.86428300	1.60701400
O	-4.24698700	0.75356200	-1.25491600
H	-3.64881600	1.05642600	-0.51712400
H	-3.58098300	0.16762400	-1.66242500
H	-5.30503100	-0.37718000	-0.39922500

Regarding the isomerization in-between the (1+1) and (2+0) structures for *cis*-$PA^{2-}(H_2O)_2$

The two water molecules are far away from each other in the (1+1) structure (i.e., iso A, Fig. 4), and we do not expect there is one transition state directly associated with the two structures of (1+1) and (2+0). We think the most likely pathway for the isomerization is that one water molecule dissociate from (2+0), followed by the attachment of water molecule onto (1+0) to form (1+1). There is no energetic barrier for the hydrogen bond dissociation and formation, and the barrier for the isomerization could be roughly estimated to be the energy difference between (1+0) + (water) and (2+0), which is predicted to be about 67 kJ/mol between isomers A and D at the M06-2X/aug-cc-pVDZ level of theory.