

Multifunctional Imidazole-Derived Polymeric Catalyst for Dephosphorylation Reactions Potentiated by Cationic and Anionic Micelles

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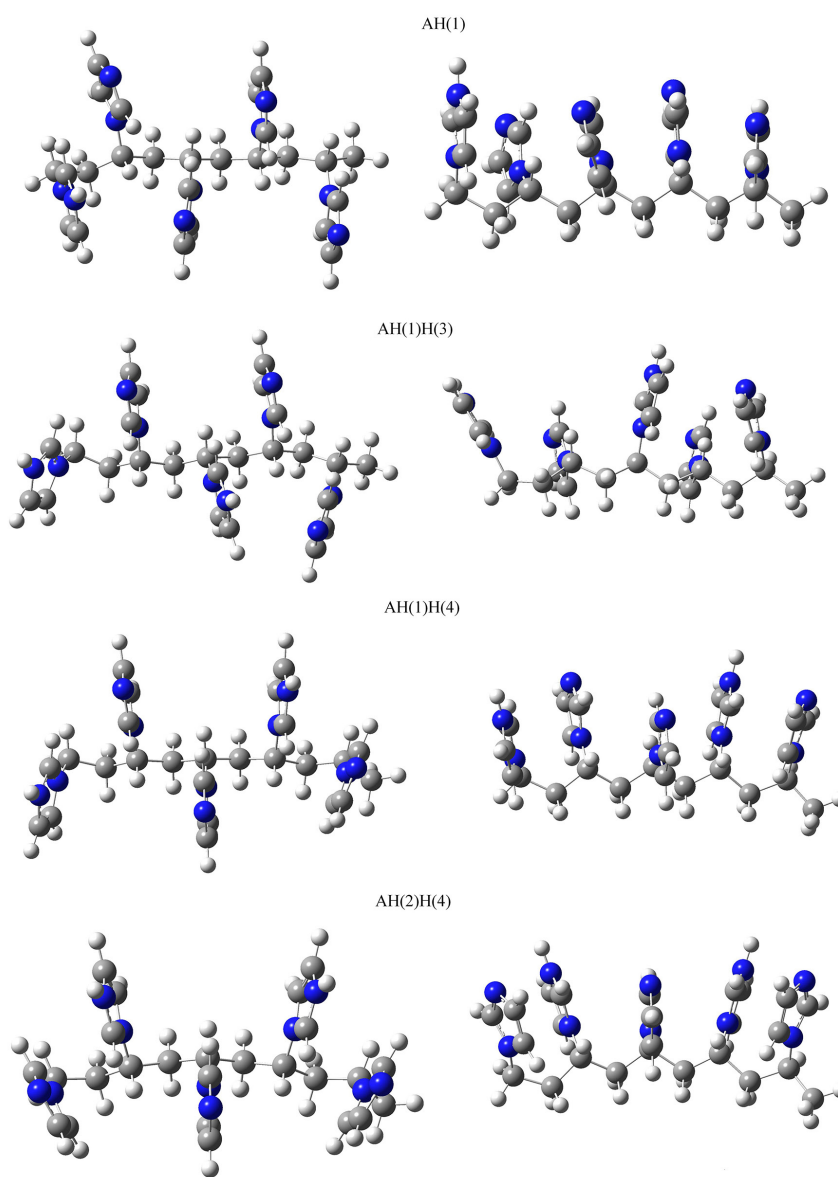


Figure S1. Optimized structures of syndiotactic PVI pentamer with single (A-H(1)) and double (A-H(1)H(3), A-H(1)H(4) and A-H(2)H(4)) protonation.

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Table S1. Optimized geometry of A-H(1) in cartesian coordinates

C	6.37705900	1.07618300	-1.32274800	C	2.20838200	2.84364500	0.57750000
H	6.46197500	0.53270800	-2.27057000	C	2.21270000	1.06395600	1.88032100
H	6.33746300	2.14763500	-1.54829400	C	1.98230900	3.19184800	1.88906400
C	5.12732500	0.65204900	-0.54062800	H	2.28886300	3.43748300	-0.32151900
H	5.08034300	1.23606700	0.38508500	H	2.29491600	0.02385800	2.16942200
C	3.83624200	0.90297500	-1.34590600	H	1.82510400	4.18078300	2.29828500
H	3.85950700	0.29642500	-2.26033200	N	-0.12280600	-0.90075200	-0.18440300
H	3.82837300	1.95161700	-1.66897100	C	-0.53068100	-1.13935300	1.10418800
C	2.53554600	0.58606100	-0.58557000	C	-0.06896800	-2.13845800	-0.80469400
H	2.60864000	-0.42803600	-0.17880600	H	-0.62468800	-0.33954800	1.82795100
C	1.31006900	0.65367900	-1.52281400	H	0.25031800	-2.26065000	-1.82951600
H	1.45102000	-0.07963900	-2.32713400	N	-3.03058200	1.62754700	-0.41725200
H	1.27153400	1.63893500	-2.00485400	C	-3.49124400	2.81633100	-0.96312900
C	-0.04260900	0.42016300	-0.82941200	C	-3.17926700	1.75360000	0.94301300
H	-0.14504800	1.15124000	-0.02035100	H	-3.47970900	3.01085900	-2.02601100
C	-1.22805400	0.58994500	-1.81044100	H	-2.85619500	0.97783500	1.62588000
H	-1.13111300	-0.15032400	-2.61411200	N	-5.03360700	-1.21780900	-0.29831700
H	-1.16871900	1.57856900	-2.27966400	C	-5.25637000	-0.89331200	0.97993800
C	-2.60117200	0.41717500	-1.12672600	C	-4.71215500	-2.56657400	-0.36418200
H	-2.48780800	-0.34484900	-0.34887500	H	-5.51863600	0.08824900	1.34807600
C	-3.69567600	-0.07452800	-2.09442000	C	-4.73857200	-3.05510000	0.90833400
H	-3.35654400	-1.01219600	-2.55017100	H	-4.49113300	-3.05875400	-1.29856400
H	-3.83731200	0.63571900	-2.91819500	H	-4.53568900	-4.04115800	1.29682300
C	-5.07198100	-0.27439500	-1.44276000	N	5.24379600	-2.52368500	1.24652900
H	-5.46346500	0.66936000	-1.05687500	N	-5.08255300	-1.99446100	1.72279200
H	-5.78963100	-0.66942800	-2.16718400	N	1.98561900	2.07517000	2.69341400
N	5.21025700	-0.75006000	-0.11312000	H	7.28021100	0.88163000	-0.73646700
C	5.19413900	-1.20877500	1.17896800	H	-5.17228400	-2.02920500	2.73297600
C	5.27936400	-1.87373100	-0.91980800	N	-0.73340400	-2.42102500	1.33984200
H	5.15687400	-0.53295000	2.02416000	C	-0.43833700	-3.05465900	0.15279900
C	5.29909800	-2.94834400	-0.06064500	H	-0.47791300	-4.13209200	0.06229800
H	5.33344400	-1.81105600	-1.99685500	N	-3.69810700	2.91244100	1.28773400
H	5.36034000	-3.99940000	-0.30954800	C	-3.89479700	3.58595600	0.10376000
N	2.35840200	1.46496300	0.57591300	H	-4.30624700	4.58601000	0.08597800

Table S2. Optimized geometry of A-H(3) in cartesian coordinates

C	6.21558900	0.02719400	-1.85212400	C	2.31726300	2.95383000	-0.17893100
H	6.08081400	-0.69330300	-2.66672300	C	2.52953300	1.56265900	1.51788700
H	6.36526100	1.01659900	-2.29748800	C	2.30550700	3.63060200	1.01930000
C	5.00519900	0.04881400	-0.91259500	H	2.25307200	3.29960300	-1.20064200
H	5.18450300	0.79037000	-0.12617800	H	2.67721500	0.62826500	2.04453500
C	3.70259200	0.41742900	-1.65808500	H	2.21544300	4.69598200	1.18203700
H	3.53480400	-0.31599400	-2.45690100	N	-0.20445600	-0.46716700	0.33885100
H	3.83860900	1.38913800	-2.14791000	C	-0.26566400	-0.12580100	1.63130300
C	2.45358600	0.45718100	-0.75517900	C	-0.18134600	-1.85363500	0.24809800
H	2.48843400	-0.41994200	-0.10063100	H	-0.29332500	0.88210800	2.02036600
C	1.15342000	0.38899600	-1.58430800	H	-0.13087900	-2.37070800	-0.69705800
H	1.16432700	-0.55084000	-2.15073200	N	-2.89319500	1.63284600	-0.21878000
H	1.14276900	1.19387600	-2.32948400	C	-2.79415300	2.94640700	-0.65222900
C	-0.16451100	0.50640400	-0.79324800	C	-3.06419200	1.69568900	1.14317900
H	-0.21086800	1.48794700	-0.31393500	H	-2.67093400	3.20689500	-1.69358700
C	-1.38945300	0.33064000	-1.71128900	H	-3.20546300	0.80377600	1.74046500
H	-1.32558600	-0.63208700	-2.23403700	N	-5.19504500	-1.29472400	-0.54670900
H	-1.31721000	1.10350300	-2.48609600	C	-5.18259900	-1.35723900	0.82297300
C	-2.76491400	0.40963500	-1.01636900	C	-4.92483400	-2.57597000	-0.99496600
H	-2.83411800	-0.41490000	-0.29814500	H	-5.39870500	-0.49110900	1.43561100
C	-3.92143100	0.24900900	-2.02298000	C	-4.76741900	-3.34209400	0.13733800
H	-3.66283800	-0.55286700	-2.72487900	H	-4.90970400	-2.82490700	-2.04668800
H	-4.03582100	1.16386400	-2.61702300	H	-4.57771100	-4.40521800	0.20213200
C	-5.27124500	-0.08367000	-1.35943500	N	4.43087300	-2.64073500	1.47939200
H	-5.59542800	0.73098800	-0.70529400	N	-4.92552600	-2.57117700	1.26765800
H	-6.03900800	-0.21061700	-2.12965500	N	2.43693200	2.75302400	2.07120000
N	4.83711600	-1.23268700	-0.21000100	H	7.12259200	-0.24292000	-1.30327200
C	4.74398700	-1.40348200	1.14689700	C	-0.23091400	-2.34704400	1.51772100
C	4.56040800	-2.46674000	-0.77314100	H	-0.23237000	-3.36069900	1.88778000
H	4.94182900	-0.59398000	1.83821300	N	-0.28348000	-1.25110300	2.35714600
C	4.31827900	-3.31437800	0.28422000	H	-0.32792600	-1.28220500	3.37048300
H	4.59671900	-2.63779700	-1.83912900	N	-3.07529100	2.93217100	1.59229700
H	4.09668500	-4.37295600	0.25215600	C	-2.90837800	3.72244900	0.47828800
N	2.45846300	1.61348700	0.14707200	H	-2.88577600	4.80127400	0.55086300

Table S3. Optimized geometry of A-H(1)H(3) in cartesian coordinates

C	6.52389800	0.46549100	-1.56953600	C	2.50483000	1.84821500	1.54827300
H	6.47368000	-0.16389800	-2.46499300	C	1.93255900	3.81452600	0.93290500
H	6.65923300	1.50209600	-1.89501100	H	2.04582200	3.38120000	-1.26681100
C	5.25701700	0.34484000	-0.71867800	H	2.81277500	0.98898500	2.13075000
H	5.35048700	1.00993600	0.14730100	H	1.65407500	4.85447100	1.03600300
C	3.98160600	0.72734200	-1.51074200	N	0.34892900	-0.91002800	0.35581400
H	3.89687900	0.05750000	-2.37517100	C	0.35315100	-0.66953900	1.67400400
H	4.09998900	1.74198900	-1.90721900	C	0.75218300	-2.22537700	0.14764200
C	2.69233200	0.63556200	-0.66529000	H	0.11722300	0.27379500	2.14613600
H	2.82569800	-0.19253500	0.03780000	H	0.86455900	-2.64846800	-0.83813000
C	1.43862000	0.32885800	-1.51111300	N	-2.72055400	1.02215900	-0.21040300
H	1.63797600	-0.56643500	-2.11285400	C	-2.79269400	2.32714000	-0.68082200
H	1.25280600	1.14341000	-2.22102000	C	-3.13137500	1.06915000	1.10139700
C	0.13997100	0.13137000	-0.69551000	H	-2.51994800	2.59994400	-1.69046600
H	-0.07394100	1.04976000	-0.14165000	H	-3.16595500	0.17998500	1.72035300
C	-1.05337100	-0.20247200	-1.61004500	N	-5.68079500	-0.73492100	-0.66055800
H	-0.89608400	-1.17128600	-2.10132800	C	-6.15251400	-0.15163700	0.44889500
H	-1.04162500	0.54358700	-2.41328800	C	-6.08596400	-2.06438600	-0.66937400
C	-2.45628500	-0.20633400	-0.95889900	H	-6.00634100	0.88059900	0.73638100
H	-2.50102000	-1.00762600	-0.21162700	C	-6.80732100	-2.27830300	0.46836800
C	-3.53546000	-0.47987600	-2.04600400	H	-5.85141700	-2.73193400	-1.48495000
H	-3.51066200	-1.54570200	-2.30411600	H	-7.30618900	-3.16130700	0.83926000
H	-3.26221000	0.05340500	-2.96566900	N	4.49939700	-2.57665800	1.32508300
C	-4.97526200	-0.02769500	-1.75719700	N	-6.83026000	-1.07283300	1.14483800
H	-5.00379500	1.03489400	-1.50795000	N	2.17589500	3.02523100	2.03340500
H	-5.57934600	-0.17134400	-2.65782500	H	7.40492600	0.17100900	-0.99203400
N	5.09832600	-1.00907900	-0.15586400	H	-7.30547400	-0.89482100	2.02487800
C	4.81190500	-1.30545900	1.15109600	C	1.00186300	-2.77558700	1.36972600
C	4.95834400	-2.19289600	-0.85796800	H	1.37083900	-3.75033900	1.64986700
H	4.88600500	-0.56045200	1.93357300	N	0.73684200	-1.79043500	2.29934600
C	4.59929300	-3.14177200	0.07239800	N	-3.45052500	2.28534200	1.48432800
H	5.16695200	-2.26775900	-1.91521300	C	-3.23946300	3.08174600	0.38039500
H	4.44802100	-4.20185600	-0.08416300	H	-3.41027900	4.14926400	0.41435500
N	2.48134500	1.81954900	0.17387500	H	0.86345500	-1.87988600	3.30307400
C	2.11425000	3.09568200	-0.22680600				

Table S4. Optimized geometry of A-H(1)H(4) in cartesian coordinates

C	-6.12544900	-0.69760800	2.36567600	C	-2.92739300	0.98472800	-1.31329400
H	-5.90060400	-1.75404000	2.54852000	C	-2.99424200	3.17472300	-0.93158200
H	-6.08022300	-0.16739000	3.32335700	H	-2.61189700	2.94978700	1.24228500
C	-5.13560300	-0.08521000	1.36626900	H	-2.98710400	0.02633100	-1.81210800
H	-5.43333000	0.95292600	1.18004700	H	-3.10338100	4.22219300	-1.16939600
C	-3.69685700	-0.08488400	1.94690100	N	0.12937900	-1.04896800	0.04853400
H	-3.52344200	-1.03377300	2.47008000	C	0.19738400	-1.07170200	-1.32441900
H	-3.65395800	0.69362000	2.71929500	C	0.11970400	-2.37638400	0.45428200
C	-2.50761500	0.06886900	0.97260300	H	0.23155000	-0.16102100	-1.91002400
H	-2.45300600	-0.82600500	0.34881500	H	0.06659100	-2.66811700	1.49358300
C	-1.18029300	0.22473200	1.74020000	N	2.81191900	1.39358100	0.13216500
H	-1.16151000	-0.57115700	2.49425300	C	2.88542300	2.73576700	0.47766000
H	-1.17567000	1.16796400	2.30101800	C	2.95719100	1.34356400	-1.23356200
C	0.10870100	0.14869100	0.89030800	H	2.80632300	3.08008500	1.49913800
H	0.13051400	0.99621700	0.19561600	H	2.91266500	0.40822200	-1.77843000
C	1.36282700	0.22659500	1.78973800	N	5.73710300	-0.53711000	0.38789300
H	1.36699300	-0.62483600	2.48165600	C	6.00017200	-0.24188300	-0.89090800
H	1.29406900	1.13003400	2.40851900	C	6.04526200	-1.87370600	0.60688800
C	2.70209400	0.23520600	1.02232100	H	5.86687400	0.72300400	-1.35972900
H	2.72722400	-0.64019600	0.36371000	C	6.49505000	-2.38734200	-0.57389000
C	3.89584800	0.15477700	2.00391400	H	5.93834500	-2.33710500	1.57599600
H	3.87898700	-0.82611500	2.49416300	H	6.84061800	-3.37666100	-0.83387800
H	3.76700100	0.89373500	2.80506400	N	-5.56823000	-0.91760900	-2.14925200
C	5.28511900	0.43435300	1.41388300	N	6.45481100	-1.35131100	-1.48731200
H	5.31670100	1.42001200	0.94477100	N	-3.09442400	2.18155800	-1.88818200
H	6.03351600	0.42149500	2.21137600	H	-7.14780900	-0.62675400	1.98356000
N	-5.21372600	-0.73391900	0.05040700	H	6.73865400	-1.40790100	-2.46074200
C	-5.70238400	-0.14658400	-1.08934800	H	-3.31088800	2.31764300	-2.87107300
C	-4.75980900	-1.98698700	-0.32650700	C	0.18010000	-3.11933200	-0.70267500
H	-6.16164700	0.83451300	-1.07440500	H	0.18507800	-4.19634800	-0.80327300
C	-4.98429100	-2.07389300	-1.68367000	N	0.22957100	-2.29577600	-1.80397700
H	-4.36467700	-2.69960100	0.38337500	N	3.11594400	2.53720100	-1.76450900
H	-4.77738200	-2.90680900	-2.34193100	C	3.07296200	3.41512700	-0.70485200
N	-2.70324100	1.17758500	-0.00739400	H	3.18042700	4.48144200	-0.85137200
C	-2.74879200	2.54304700	0.25232400				

Table S5. Optimized geometry of A-H(2)H(4) in cartesian coordinates

C	-5.97274900	-0.79260400	2.47640700	C	-3.05929500	1.02781800	-1.33969500
H	-5.66029600	-1.82474800	2.66895500	C	-3.32454100	3.21165100	-1.01157900
H	-5.93676700	-0.24169300	3.42271900	H	-2.81870000	3.09249300	1.14543700
C	-5.06915100	-0.12465600	1.43172400	H	-3.05298100	0.05223500	-1.80872100
H	-5.45390100	0.88335200	1.23954900	H	-3.55601600	4.23449300	-1.26885600
C	-3.61597100	-0.00041000	1.96244200	N	0.19237000	-0.72015300	-0.04218300
H	-3.35386400	-0.92126800	2.49852800	C	0.24996200	-0.68523100	-1.41625900
H	-3.60922200	0.79611500	2.71734900	C	0.18243900	-2.06453000	0.30616500
C	-2.46991200	0.22214800	0.94795500	H	0.26697900	0.24987100	-1.96399700
H	-2.36185000	-0.68230200	0.34566100	H	0.14045000	-2.40096800	1.33258900
C	-1.14174500	0.49384500	1.68240400	N	3.16463900	1.19886200	0.12766000
H	-1.07274700	-0.26747900	2.46848600	C	3.33670800	2.56924800	0.29325300
H	-1.18449100	1.45688800	2.20713400	C	3.51695700	0.87336300	-1.12318800
C	0.15690700	0.44638800	0.83653100	H	3.13967400	3.06980400	1.22877400
H	0.17955000	1.31312000	0.16477900	H	3.52744100	-0.12499500	-1.54089100
C	1.38895500	0.50471600	1.77754400	N	5.51692400	-0.86866400	0.60638400
H	1.25227000	-0.23129100	2.57886400	C	6.15825900	-0.40178200	-0.51402200
H	1.40413600	1.48320300	2.27447400	C	5.03383000	-2.12525800	0.28021300
C	2.76695100	0.19630100	1.15878000	H	6.67387600	0.55102000	-0.52105000
H	2.70112800	-0.74004400	0.60036700	C	5.39833700	-2.33567700	-1.03204500
C	3.83362600	0.02924900	2.26605400	H	4.53099700	-2.75671800	0.99912200
H	3.53540500	-0.86677800	2.82278600	H	5.21986200	-3.21072800	-1.64212500
H	3.77444800	0.85905700	2.98210700	N	-5.56040500	-1.05447000	-2.05120800
C	5.31247100	-0.10816700	1.83437600	N	6.09377100	-1.25117200	-1.51780900
H	5.75451400	0.87780600	1.66355100	N	-3.37174800	2.18422100	-1.93596500
H	5.87096200	-0.56521400	2.65858300	H	-7.00996800	-0.80859500	2.12990800
N	-5.14097700	-0.80203300	0.13025900	H	-3.66282600	2.26440100	-2.90592300
C	-5.71931400	-0.27808600	-0.99868600	N	3.88179300	1.99342100	-1.75747000
C	-4.59993100	-2.02064100	-0.24474000	C	3.78711200	3.06919000	-0.89363200
H	-6.26012300	0.66053800	-0.98018700	H	4.04737300	4.07477100	-1.18872400
C	-4.86636000	-2.15039100	-1.59114300	H	4.23408400	2.01976500	-2.71002000
H	-4.12673100	-2.68803500	0.46133500	N	0.27723800	-1.88652600	-1.94737900
H	-4.61743100	-2.97610000	-2.24395900	C	0.23559400	-2.75692800	-0.88254700
N	-2.78665000	1.28258800	-0.05323000	H	0.24607400	-3.82842700	-1.02982900
C	-2.95747100	2.64443400	0.17365600				