Supporting information

Novel pyrimethamine salts with isomeric dihydroxybenzoic acids - crystallization and characterization

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1. Cartesian coordinates of obtained structures

Structure:	**PYR/23DHBA (mode A)**		
Level of theory:	DFT/M06-2X/Def2-TZVP		
E(RM062X):		-1715.657616	Hartree
E+Thermal Free Energy Corr.:		-1715.351927	Hartree
Number of negative frequencies:			0
Atom	**X**	**Y**	**Z**
H	4.454100	2.571000	-0.042900
H	-1.887700	2.667300	0.011200
H	-1.323500	0.290900	-0.000600
H	3.535600	4.041500	0.070700
H	-0.908600	4.124500	0.120300
C	0.145100	2.406100	0.045600
C	2.412800	2.355200	0.046500
C	2.407200	0.939000	-0.045100
C	1.161500	0.346600	-0.080700
C	0.978800	-1.145200	-0.095500
H	1.856100	-1.625800	-0.524700
H	0.119700	-1.386200	-0.722600
C	0.743600	-1.667300	1.324700
H	1.602800	-1.447500	1.960500
H	0.592300	-2.746100	1.314400
H	-0.139600	-1.202300	1.762500
C	3.683900	0.182500	-0.083400
C	4.461800	0.046400	1.066600
H	4.113300	0.482400	1.995300
C	5.667100	-0.639600	1.041300
H	6.264300	-0.748000	1.936100
C	6.101700	-1.198500	-0.150200
C	5.351700	-1.076100	-1.309700
H	5.709100	-1.516100	-2.230400
C	4.152400	-0.381800	-1.269600
H	3.564100	-0.276600	-2.173100
N	0.029900	1.070100	-0.031500
N	-0.986700	3.124900	0.088100
N	1.300000	3.074200	0.085200
N	3.577900	3.038000	0.106900
Cl	7.604000	-2.058900	-0.192500
C	-4.471400	-0.641000	-0.027900
C	-5.739700	-0.066400	-0.116100
C	-6.878100	-0.884400	-0.100200
C	-6.741200	-2.251800	0.003500
H	-7.636600	-2.859400	0.013800
C	-5.472300	-2.826700	0.092500

H	-5.378100	-3.900700	0.173800
C	-4.347500	-2.031800	0.076800
H	-3.357700	-2.459300	0.145100
C	-3.284200	0.236700	-0.046400
O	-2.136200	-0.368700	0.032100
O	-3.388900	1.464100	-0.130700
O	-5.971500	1.257400	-0.219800
H	-5.095900	1.701500	-0.217400
O	-8.104900	-0.317000	-0.187200
H	-7.985300	0.639800	-0.251000

Structure:	**PYR/23DHBA (mode B)**		
Level of theory:	DFT/M06-2X/Def2-TZVP		
E(RM062X):		-1715.653870	Hartree
E+Thermal Free Energy Corr.:		-1715.348160	Hartree
Number of negative frequencies:			0
Atom	X	Y	Z
H	4.479300	2.475500	0.049100
H	-1.832800	3.130800	-0.029800
H	-1.432500	0.737400	-0.071900
H	3.689500	4.017500	0.186700
H	-0.728200	4.490600	0.142800
C	0.169800	2.691000	0.040400
C	2.424900	2.438200	0.085700
C	2.298800	1.029300	-0.046900
C	1.008100	0.551100	-0.123700
C	0.690900	-0.917200	-0.188600
H	1.538400	-1.466800	-0.593800
H	-0.153700	-1.060000	-0.864400
C	0.344300	-1.454500	1.203100
H	1.197500	-1.351000	1.875100
H	0.077300	-2.509700	1.150700
H	-0.496000	-0.907500	1.631400
C	3.505200	0.165000	-0.079200
C	4.249700	-0.053600	1.080200
H	3.926000	0.399100	2.009900
C	5.390800	-0.841900	1.062900
H	5.961900	-1.013800	1.964800
C	5.793500	-1.422100	-0.129700
C	5.075600	-1.219600	-1.298300
H	5.407100	-1.678100	-2.219700

C	3.941300	-0.422900	-1.266300
H	3.379500	-0.254600	-2.177100
N	-0.056600	1.370700	-0.075600
N	-0.894100	3.503100	0.079100
N	1.379300	3.250800	0.122000
N	3.643100	3.013600	0.188300
Cl	7.213700	-2.411900	-0.160600
C	-4.688200	0.101100	-0.114000
C	-4.710300	-1.287900	0.015300
C	-5.938000	-1.965100	0.028800
C	-7.118800	-1.263200	-0.085900
H	-8.049000	-1.815800	-0.072200
C	-7.097200	0.125000	-0.215200
H	-8.027600	0.668600	-0.304600
C	-5.896000	0.798800	-0.228100
H	-5.850200	1.874300	-0.326000
C	-3.427800	0.885400	-0.133400
O	-2.323600	0.157100	-0.048000
O	-3.407300	2.095500	-0.219400
O	-3.623000	-2.086200	0.137100
H	-2.830700	-1.521600	0.111400
O	-5.952500	-3.314500	0.155900
H	-5.037500	-3.616400	0.223000

Structure:	**PYR/24DHBA (mode A)**		
Level of theory:	DFT/M06-2X/Def2-TZVP		
E(RM062X):		-1715.640008	Hartree
E+Thermal Free Energy Corr.:		-1715.334512	Hartree
Number of negative frequencies:			0
Atom	X	Y	Z
C	4.536400	-0.245700	-0.080400
C	4.448700	-1.635700	-0.152400
C	5.563900	-2.444800	-0.225200
H	5.465700	-3.521900	-0.279900
C	6.822900	-1.850500	-0.227100
C	6.947200	-0.473200	-0.157000
H	7.938300	-0.036000	-0.160400
C	5.817100	0.333800	-0.083600
C	3.295200	0.566200	-0.003400
O	3.278700	1.776400	0.074500
O	2.193700	-0.167400	-0.027200

O	7.968100	-2.571300	-0.296200
H	7.758200	-3.509300	-0.342800
C	-0.290500	2.503000	0.104100
C	-2.552800	2.354000	0.011800
C	-2.487200	0.935900	0.013600
C	-1.212600	0.400100	0.063200
C	-0.948500	-1.081200	0.076100
H	-1.841300	-1.624200	-0.229700
H	-0.165800	-1.285400	-0.657500
C	-0.479000	-1.559200	1.451900
H	-1.240300	-1.378000	2.211700
H	-0.267300	-2.628000	1.431000
H	0.429800	-1.037400	1.749100
C	-3.726000	0.123200	-0.044500
C	-4.109700	-0.692600	1.019400
H	-3.491600	-0.727700	1.907600
C	-5.267000	-1.454600	0.962500
H	-5.556400	-2.088300	1.789400
C	-6.063300	-1.391500	-0.169700
C	-5.715400	-0.581200	-1.239300
H	-6.346200	-0.548300	-2.116900
C	-4.550600	0.167500	-1.170400
H	-4.268400	0.794700	-2.007500
N	-0.116700	1.171900	0.106200
N	0.805600	3.272500	0.153200
N	-1.475800	3.121400	0.061500
N	-3.746900	2.995500	-0.055100
Cl	-7.513900	-2.335800	-0.249800
H	-4.598900	2.489500	0.110400
H	1.730100	2.850700	0.144100
H	0.683500	4.267300	0.113600
H	-3.735500	3.989100	0.099600
H	1.363700	0.422800	0.031000
H	3.463500	-2.079300	-0.150000
O	5.946500	1.673100	-0.016500
H	6.881900	1.900600	-0.031300

Structure:	**PYR/24DHBA (mode B)**	
Level of theory:	DFT/M06-2X/Def2-TZVP	
E(RM062X):	-1715.654128	Hartree

E+Thermal Free Energy Corr.:	-1715.348166	Hartree
Number of negative frequencies:		0
Atom	X	Y	Z
C	4.569900	0.020700	-0.087000
C	4.619000	-1.383600	-0.116800
C	5.850600	-2.035300	-0.146700
H	5.862800	-3.118500	-0.169200
C	7.022300	-1.299500	-0.147800
C	6.994100	0.095800	-0.118700
H	7.925900	0.643000	-0.120300
C	5.772200	0.729600	-0.088200
H	5.711300	1.809600	-0.064100
C	3.283300	0.764800	-0.050300
O	3.280500	2.000400	-0.008000
O	2.204800	0.053900	-0.062100
O	3.514500	-2.144300	-0.116500
H	2.758000	-1.510900	-0.103400
O	8.242600	-1.895900	-0.176900
H	8.132900	-2.851500	-0.195100
C	-0.189700	2.585400	0.101600
C	-2.456400	2.388100	0.092500
C	-2.384200	0.961100	0.013300
C	-1.122900	0.428100	-0.011200
C	-0.813200	-1.037400	-0.081800
H	-1.703500	-1.579100	-0.395900
H	-0.042800	-1.180200	-0.842700
C	-0.298900	-1.575600	1.257200
H	-1.049600	-1.461500	2.040000
H	-0.059700	-2.634200	1.164500
H	0.605900	-1.051000	1.561800
C	-3.619800	0.141700	-0.038300
C	-3.985000	-0.678300	1.027900
H	-3.357300	-0.713400	1.909500
C	-5.139100	-1.445300	0.978800
H	-5.416800	-2.084100	1.805700
C	-5.946500	-1.382700	-0.146100
C	-5.612700	-0.568100	-1.217600
H	-6.251200	-0.537600	-2.089600
C	-4.451700	0.186900	-1.157800
H	-4.178600	0.814300	-1.998000
N	-0.044200	1.241900	0.036900
N	0.908700	3.323000	0.132700
N	-1.387900	3.169700	0.135000
N	-3.651700	3.002500	0.128400

Cl	-7.390400	-2.332800	-0.215300
H	-4.506000	2.476100	0.171400
H	1.850600	2.881700	0.085200
H	0.790200	4.320000	0.171500
H	-3.669000	4.002200	0.233600
H	0.973000	0.781500	-0.005900

Structure:	**PYR/25DHBA (mode A)**		
Level of theory:	DFT/M06-2X/Def2-TZVP		
E(RM062X):		-1715.651541	Hartree
E+Thermal Free Energy Corr.:		-1715.346117	Hartree
Number of negative frequencies:			0
Atom	X	Y	Z
C	4.597200	-0.240200	-0.082300
C	4.508300	-1.631000	-0.178200
C	5.648200	-2.403400	-0.238600
C	6.896500	-1.783500	-0.203000
H	7.797700	-2.385600	-0.250300
C	6.998200	-0.410600	-0.108100
C	5.854100	0.383400	-0.046000
C	3.366400	0.576600	-0.018500
O	3.405800	1.805000	0.067500
O	2.249200	-0.092000	-0.059000
H	0.790100	4.332700	0.069200
H	-3.633300	4.033200	0.057000
H	-4.486800	2.523200	0.071100
H	1.841700	2.922900	0.102300
H	1.407000	0.521600	-0.002800
C	-0.176600	2.562500	0.061700
C	-2.438100	2.402700	-0.009300
C	-2.365400	0.984100	-0.003100
C	-1.091500	0.452000	0.034600
C	-0.825300	-1.028200	0.051300
H	-1.718100	-1.569400	-0.257900
H	-0.040000	-1.236700	-0.677800
C	-0.366600	-1.505500	1.431200
H	-1.137000	-1.329500	2.182900
H	-0.149400	-2.572900	1.409600
H	0.537100	-0.981400	1.739500
C	-3.602500	0.166600	-0.043000
C	-3.995200	-0.605800	1.049300

H	-3.386200	-0.603900	1.944500
C	-5.151000	-1.371100	1.010900
H	-5.448100	-1.971900	1.859400
C	-5.935200	-1.355300	-0.131500
C	-5.577400	-0.587800	-1.229200
H	-6.199300	-0.591300	-2.113800
C	-4.414700	0.165600	-1.178300
H	-4.124400	0.759000	-2.036900
N	0.002900	1.232200	0.065100
N	0.917000	3.338100	0.097600
N	-1.362800	3.175000	0.027500
N	-3.633400	3.035200	-0.063900
Cl	-7.382000	-2.305400	-0.188900
O	5.502600	-3.759200	-0.331800
H	6.368300	-4.175600	-0.366600
O	6.018000	1.713700	0.046100
H	5.127700	2.115500	0.079600
H	3.537400	-2.104700	-0.205600
H	7.962500	0.078000	-0.079600

Structure:	**PYR/25DHBA (mode B)**		
Level of theory:	DFT/M06-2X/Def2-TZVP		
E(RM062X):		-1715.648847	Hartree
E+Thermal Free Energy Corr.:		-1715.342741	Hartree
Number of negative frequencies:			0
Atom	X	Y	Z
C	4.567900	-0.336700	-0.095300
C	4.549400	-1.736300	-0.111300
C	5.761400	-2.429100	-0.151800
H	5.731000	-3.510400	-0.163200
C	6.961900	-1.752100	-0.177000
H	7.902200	-2.287000	-0.209200
C	6.981700	-0.358400	-0.161900
C	5.792200	0.335900	-0.120600
H	5.771100	1.419700	-0.106300
C	3.313700	0.475200	-0.047900
O	3.382200	1.709400	-0.013300
O	2.204700	-0.177400	-0.042900
O	3.411200	-2.459300	-0.087700
H	2.679800	-1.805400	-0.073600
O	8.204900	0.256100	-0.189000

H	8.078300	1.209100	-0.176400
H	1.007800	4.154200	0.209200
H	-3.461000	4.067100	0.274400
H	-4.376300	2.587200	0.198600
H	1.991800	2.665700	0.106300
H	1.003800	0.614800	0.014000
C	-0.060700	2.472800	0.130800
C	-2.334200	2.393300	0.120700
C	-2.336200	0.965100	0.029000
C	-1.104600	0.367000	0.001900
C	-0.870200	-1.111600	-0.078900
H	-1.786700	-1.604700	-0.397700
H	-0.106900	-1.288600	-0.839900
C	-0.385900	-1.685000	1.256900
H	-1.129900	-1.536300	2.040200
H	-0.203100	-2.754100	1.157100
H	0.545300	-1.211400	1.565400
C	-3.613400	0.213100	-0.035200
C	-4.026600	-0.599100	1.019300
H	-3.404800	-0.680300	1.902000
C	-5.221600	-1.299900	0.957400
H	-5.537100	-1.932800	1.775300
C	-6.020900	-1.177800	-0.168400
C	-5.638600	-0.369800	-1.228700
H	-6.271600	-0.292700	-2.101800
C	-4.437600	0.318400	-1.156300
H	-4.127200	0.940100	-1.987700
N	0.014700	1.124300	0.057400
N	1.074900	3.152700	0.165700
N	-1.226300	3.118200	0.169400
N	-3.495500	3.068500	0.162900
Cl	-7.516000	-2.043500	-0.253300

Structure:	**PYR/26DHBA (mode A/B)**
Level of	DFT/M06-2X/Def2-TZVP

theory:			
E(RM062X):		-1715.663209	Hartree
E+Thermal Free Energy Corr.:		-1715.355569	Hartree
Number of negative frequencies:			0
Atom	X	Y	Z
H	-4.263500	2.594300	0.196500
H	1.137900	4.117100	0.207400
H	-3.336700	4.067500	0.275300
H	2.098900	2.622400	0.099200
H	1.080300	0.590200	0.006800
C	0.049400	2.445500	0.127600
C	-2.224000	2.384400	0.122900
C	-2.238500	0.955800	0.028300
C	-1.014200	0.346100	-0.003700
C	-0.790600	-1.133500	-0.087600
H	-0.029400	-1.315200	-0.849500
H	-1.711400	-1.618200	-0.406700
C	-0.310700	-1.713200	1.247300
H	0.622700	-1.246000	1.559000
H	-0.133100	-2.782600	1.143900
H	-1.055200	-1.563200	2.029800
C	-3.522800	0.215400	-0.032700
C	-3.946100	-0.582200	1.028900
H	-3.327500	-0.661000	1.914000
C	-5.147900	-1.271500	0.970400
H	-5.471900	-1.893200	1.793600
C	-5.943000	-1.152600	-0.158900
C	-5.549900	-0.358900	-1.226100
H	-6.179800	-0.284100	-2.101700
C	-4.342400	0.318300	-1.157200
H	-4.023800	0.928800	-1.993800
N	0.111500	1.096800	0.050900
N	1.192000	3.114800	0.161600
N	-1.108900	3.100000	0.169900
N	-3.378200	3.068400	0.170500
Cl	-7.445900	-2.004000	-0.239300
C	4.666600	-0.448100	-0.106700
C	5.933000	0.180300	-0.131100
C	7.097500	-0.579400	-0.172400
H	8.047700	-0.065200	-0.191000
C	7.007700	-1.960000	-0.187600
H	7.917000	-2.547800	-0.219400
C	5.785000	-2.609900	-0.163200
H	5.707600	-3.687700	-0.174700

C	4.615500	-1.860900	-0.123300
C	3.431000	0.364500	-0.061900
O	2.306300	-0.243800	-0.051400
O	3.505600	1.617500	-0.033200
O	6.058600	1.513200	-0.116100
H	5.146600	1.882700	-0.082300
O	3.450000	-2.527800	-0.099900
H	2.741900	-1.846600	-0.083300