

Table S1. Chemical Shifts for the b-R(61,2) Adduct

	H1'	H2'	H2''	H3'	H4'	H5'	H5''	A2	H5	H6	H8	CH3
C1	5.68	1.79	2.29	4.64	4.02	3.66	-		5.83	7.54		
G2	5.41	2.65	2.70	4.94	4.26	3.92	-				7.86	
G3	5.63	2.63	2.75	5.00	4.37	4.09	4.17				7.76	
A4	6.11	2.49	2.78	4.97	4.42	4.17	-	7.75			8.02	
C5	5.39	1.81	2.26	4.77	4.08	4.05	-		4.54	6.82		
A6*	5.71	2.66	2.75	5.00	4.32	4.10	4.03	6.95			8.22	
A7	6.00	2.58	2.83	5.02	4.41	4.10	4.17	7.53			8.04	
G8	5.28	2.46	2.58	4.94	4.28	4.14	-				7.59	
A9	5.88	2.55	2.82	4.99	4.38	4.14	4.18	7.29			8.00	
A10	5.99	2.52	2.82	4.98	4.39	4.18	-	7.63			7.97	
G11	5.94	2.31	2.23	4.57	4.24	4.13	4.09				7.53	
C12	5.83	2.57	2.27	4.62	4.07	3.78	-		5.90	7.85		
T13	6.17	2.23	2.60	4.87	4.25	4.07	-			7.63		1.65
T14	6.10	2.21	2.54	4.87	4.21	4.13	-			7.43		1.60
C15	5.96	2.09	2.52	4.78	4.16	-	-		5.56	7.56		
T16	6.08	2.14	2.64	4.87	4.21	-	-			7.48		1.66
T17	5.74	2.17	2.50	4.86	4.14	4.11	4.20			7.38		1.73
G18	5.87	2.53	2.70	4.85	4.35	4.11	-				7.80	
T19	6.02	2.15	2.50	4.86	4.23	4.11	4.18			7.30		1.29
C20	5.91	2.10	2.38	4.78	4.12	4.06	-		5.61	7.53		
C21	5.59	1.97	2.30	4.79	4.08	4.04	-		5.67	7.46		
G22	6.14	2.62	2.35	4.66	4.16	4.04	-				7.93	

Table S2. Chemical Shifts for the b-S(61,2) adduct

	H1'	H2'	H2''	H3'	H4'	H5'	H5''	A2	H5	H6	H8	CH3
C1	5.67	1.80	2.31	4.65	4.02	3.66	-		5.81	7.54		
G2	5.41	2.66	2.70	4.95	4.27	3.92	-				7.88	
G3	5.66	2.65	2.78	5.02	4.39	4.16	4.09				7.78	
A4	6.12	2.49	2.77	4.98	4.42	4.17	-	7.74			8.05	
C5	5.36	1.73	2.16	4.74	4.08	3.88	-		4.83	6.65		
A6*	5.64	2.62	2.70	5.01	4.32	4.10	4.03	6.92			8.15	
A7	6.07	2.64	2.88	5.04	4.45	4.16	4.06	7.59			8.11	
G8	5.20	2.48	2.57	4.99	4.28	4.15	-				7.62	
A9	5.90	2.57	2.85	5.00	4.41	4.15	-	7.26			8.02	
A10	5.99	2.53	2.84	4.98	4.40	4.18	-	7.61			7.98	
G11	5.92	2.31	2.21	4.57	4.05	4.24	4.24				7.52	
C12	5.78	2.29	2.57	4.60	4.06	3.77	-		5.86	7.84		1.64
T13	6.16	2.22	2.58	4.87	4.26	4.06	-			7.65		1.56
T14	6.12	2.21	2.57	4.87	4.22	4.10	-			7.42		
C15	5.96	2.11	2.52	4.80	4.18	-	-		5.54	7.60		1.63
T16	6.09	2.12	2.66	4.88	4.23	4.08	-			7.49		1.74
T17	5.80	2.21	2.58	4.88	4.23	4.10	-			7.42	7.75	
G18	5.84	2.48	2.67	4.82	4.32	4.21	4.13					1.26
T19	6.02	2.15	2.49	4.85	4.24	4.15	4.11			7.33		
C20	5.91	2.10	2.38	4.80	4.12	4.02	-		5.60	7.54		
C21	5.54	1.98	2.30	4.80	4.07	4.02	-		5.67	7.47		
G22	6.14	2.63	2.35	4.67	4.17	4.04	-				7.94	

Table S3. Restraints for the b-S(61,2) adduct

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set message=off echo=off end
assign ( resid 1 and name H3' )( resid 1 and name H6 ) 3.55 0.80 0.80 !170
assign (( resid 1 and name H5' ) or ( resid 1 and name H5" ))
      ( resid 1 and name H6 ) 3.58 0.86 0.87 !84
assign ( resid 1 and name H5 )( resid 1 and name H2' ) 3.50 0.74 0.74 !277
assign ( resid 1 and name H2' )( resid 1 and name H1' ) 2.40 0.52 0.52 !278
assign ( resid 1 and name H3' )( resid 1 and name H1' ) 3.03 0.90 0.90 !363
!assign (( resid 1 and name H5' ) or ( resid 1 and name H5" ))
!      ( resid 1 and name H1' ) 2.45 0.47 0.47 !356
assign ( resid 1 and name H3' )( resid 1 and name H2' ) 2.40 0.44 0.44 !400
assign ( resid 1 and name H4' )( resid 1 and name H2' ) 3.50 0.40 0.41 !403
assign (( resid 1 and name H5' ) or ( resid 1 and name H5" ))
      ( resid 1 and name H2' ) 3.53 0.71 0.71 !405
assign (( resid 1 and name H5' ) or ( resid 1 and name H5" ))
      ( resid 1 and name H3' ) 2.69 0.54 0.54 !443
assign (( resid 1 and name H5' ) or ( resid 1 and name H5" ))
      ( resid 1 and name H4' ) 2.19 0.30 0.31 !450
assign ( resid 2 and name H8 )( resid 1 and name H1' ) 3.87 0.81 0.80 !210
assign ( resid 2 and name H8 )( resid 1 and name H2' ) 2.54 0.35 0.35 !8
!assign ( resid 2 and name H8 )( resid 1 and name H4' ) 4.07 0.77 0.78 !109
!assign ( resid 2 and name H8 )( resid 1 and name H6 ) 3.31 0.85 0.85 !254
assign ( resid 2 and name H8 )( resid 2 and name H1' ) 3.20 1.00 1.00 !204
assign ( resid 2 and name H3' )( resid 2 and name H8 ) 3.15 0.80 0.80 !151
assign ( resid 2 and name H8 )( resid 2 and name H4' ) 4.15 0.84 0.83 !114
assign (( resid 2 and name H5' ) or ( resid 2 and name H5" ))
      ( resid 2 and name H8 ) 4.53 0.98 0.97 !110
assign ( resid 2 and name H1' )( resid 2 and name H4' ) 2.77 0.50 0.50 !338
assign ( resid 3 and name H8 )( resid 2 and name H1' ) 2.67 0.29 0.29 !203
assign ( resid 3 and name H8 )( resid 2 and name H3' ) 4.55 0.61 0.62 !152
assign ( resid 3 and name H8 )( resid 3 and name H1' ) 3.20 0.77 0.76 !211
assign ( resid 3 and name H3' )( resid 3 and name H8 ) 3.16 0.80 0.80 !155
assign ( resid 3 and name H8 )( resid 3 and name H4' ) 4.70 0.66 0.65 !103
assign ( resid 3 and name H1' )( resid 3 and name H4' ) 3.20 0.29 0.29 !340
assign ( resid 3 and name H1' )( resid 4 and name H4' ) 4.20 0.30 0.30 !340
assign ( resid 3 and name H4' )( resid 3 and name H2' ) 3.52 0.56 0.56 !427
assign ( resid 4 and name H8 )( resid 3 and name H8 ) 3.57 1.00 1.00 !250
assign ( resid 4 and name H8 )( resid 4 and name H1' ) 3.40 1.06 1.06 !221
assign ( resid 4 and name H2 )( resid 4 and name H1' ) 4.58 0.58 0.58 !217
assign ( resid 4 and name H2' )( resid 4 and name H1' ) 2.21 0.35 0.35 !322
assign ( resid 4 and name H3' )( resid 4 and name H1' ) 3.70 0.77 0.76 !386
assign ( resid 4 and name H2 )( resid 5 and name H1' ) 3.69 0.37 0.37 !202
assign ( resid 4 and name H2 )( resid 20 and name H1' ) 3.84 0.38 0.38 !216
assign ( resid 5 and name H6 )( resid 4 and name H1' ) 3.30 0.50 0.50 !185
assign ( resid 5 and name H6 )( resid 4 and name H2' ) 3.03 0.54 0.54 !80
assign ( resid 5 and name H6 )( resid 4 and name H2" ) 2.71 0.50 0.50 !81
assign ( resid 5 and name H6 )( resid 4 and name H3' ) 3.83 0.76 0.75 !143

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assign ( resid 5 and name H6 )( resid 4 and name H8 ) 4.04 0.83 0.83 !247
assign ( resid 5 and name H5 )( resid 4 and name H8 ) 3.27 0.44 0.44 !149
assign ( resid 5 and name H5 )( resid 4 and name H2" ) 3.00 0.70 0.69 !434
assign ( resid 5 and name H6 )( resid 5 and name H1' ) 3.61 0.40 0.40 !144
assign ( resid 5 and name H2' )( resid 5 and name H6 ) 2.00 0.23 0.23 !78
assign ( resid 5 and name H2" )( resid 5 and name H6 ) 3.00 0.37 0.37 !79
assign ( resid 5 and name H3' )( resid 5 and name H6 ) 3.29 0.80 0.80 !141
assign ( resid 5 and name H6 )( resid 5 and name H4' ) 4.38 0.80 0.81 !140
assign ( resid 5 and name H5 )( resid 5 and name H2' ) 3.51 0.57 0.58 !397
assign ( resid 5 and name H2' )( resid 5 and name H1' ) 2.75 0.47 0.47 !279
assign ( resid 5 and name H2" )( resid 5 and name H1' ) 2.19 0.22 0.22 !293
assign ( resid 5 and name H3' )( resid 5 and name H1' ) 3.43 0.81 0.81 !379
assign ( resid 5 and name H3' )( resid 5 and name H2' ) 2.43 0.25 0.25 !398
assign ( resid 5 and name H4' )( resid 5 and name H2' ) 3.80 0.67 0.68 !402
assign ( resid 6 and name H8 )( resid 5 and name H1' ) 2.67 0.27 0.27 !205
assign ( resid 6 and name H8 )( resid 5 and name H2' ) 3.44 0.43 0.43 !5
assign ( resid 6 and name H8 )( resid 5 and name H2" ) 2.92 0.60 0.60 !6
assign ( resid 6 and name H8 )( resid 5 and name H3' ) 3.92 1.00 1.00 !148
assign ( resid 6 and name H8 )( resid 5 and name H6 ) 4.50 0.97 0.97 !246
assign ( resid 6 and name HB' )( resid 5 and name H5 ) 3.54 0.46 0.46 !433
assign ( resid 6 and name HB" )( resid 5 and name H5 ) 3.40 0.31 0.31 !446
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS5 ) or
      ( resid 6 and name HS2 ) or ( resid 6 and name HS4 ))
      ( resid 5 and name H6 ) 5.00 0.62 0.62 !261
assign ( resid 6 and name H8 )( resid 6 and name H4' ) 4.43 0.76 0.76 !119
assign ( resid 6 and name H2 )( resid 6 and name H1' ) 4.26 0.43 0.43 !188
assign ( resid 6 and name H1' )( resid 6 and name H4' ) 3.13 0.31 0.31 !339
assign ( resid 6 and name HA )( resid 6 and name HB" ) 2.80 0.50 0.50 !432
assign ( resid 6 and name HA )( resid 6 and name HB' ) 2.50 0.22 0.22 !445
assign ( resid 6 and name HB' )( resid 6 and name HB" ) 1.94 0.19 0.19 !408
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS5 ) or
      ( resid 6 and name HS2 ) or ( resid 6 and name HS4 ))
      ( resid 6 and name HB" ) 3.58 0.36 0.36 !53
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS5 ))
      ( resid 6 and name HB' ) 3.40 0.48 0.48 !85
!assign ( resid 6 and name H8 )( resid 6 and name HS1 ) 4.17 0.42 0.42 !248
assign ( resid 6 and name H2 )( resid 18 and name H1' ) 3.50 0.35 0.35 !187
assign ( resid 7 and name H8 )( resid 7 and name H1' ) 3.14 0.80 0.80 !222
assign ( resid 7 and name H2' )( resid 7 and name H8 ) 3.50 0.34 0.34 !17
assign ( resid 7 and name H8 )( resid 7 and name H4' ) 4.00 0.65 0.65 !118
assign ( resid 7 and name H5' )( resid 7 and name H8 ) 3.68 1.02 1.02 !125
assign ( resid 7 and name H5" )( resid 7 and name H8 ) 4.01 0.73 0.73 !126
assign ( resid 7 and name H2" )( resid 7 and name H1' ) 2.08 0.25 0.25 !321
assign ( resid 7 and name H3' )( resid 7 and name H1' ) 3.59 0.68 0.68 !385
assign ( resid 7 and name H4' )( resid 7 and name H2' ) 3.73 0.65 0.65 !426
assign ( resid 7 and name H4' )( resid 7 and name H2" ) 3.21 0.67 0.67 !430

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assign ( resid 7 and name H2 )( resid 17 and name H1' ) 3.79 0.38 0.38 !230
assign ( resid 8 and name H8 )( resid 7 and name H2'' ) 2.50 0.40 0.40 !34
assign ( resid 8 and name H8 )( resid 7 and name H3' ) 4.82 0.81 0.81 !156
assign ( resid 8 and name H8 )( resid 7 and name H8 ) 3.68 0.60 0.60 !249
assign ( resid 8 and name H3' )( resid 8 and name H8 ) 3.86 0.61 0.61 !157
assign ( resid 8 and name H3' )( resid 8 and name H1' ) 3.90 0.36 0.36 !381
assign ( resid 8 and name H1' )( resid 8 and name H4' ) 3.00 0.80 0.80 !336
assign (( resid 9 and name H5' ) or ( resid 9 and name H5'' ))
      ( resid 8 and name H1' ) 3.19 0.33 0.33 !337
assign ( resid 9 and name H8 )( resid 8 and name H1' ) 2.69 0.35 0.35 !160
assign ( resid 9 and name H8 )( resid 8 and name H8 ) 3.69 1.01 1.00 !251
assign ( resid 9 and name H2 )( resid 9 and name H1' ) 4.25 0.43 0.43 !189
assign ( resid 9 and name H2'' )( resid 9 and name H1' ) 2.13 0.22 0.22 !319
assign ( resid 9 and name H3' )( resid 9 and name H1' ) 3.90 0.34 0.34 !383
assign ( resid 10 and name H3' )( resid 9 and name H1' ) 4.90 0.34 0.34 !383
assign ( resid 9 and name H1' )( resid 9 and name H4' ) 3.70 0.28 0.28 !342
assign ( resid 9 and name H1' )( resid 10 and name H4' ) 4.20 0.28 0.28 !342
assign ( resid 10 and name H8 )( resid 10 and name H1' ) 3.52 0.56 0.56 !220
assign ( resid 10 and name H2'' )( resid 10 and name H1' ) 2.25 0.23 0.23 !320
assign ( resid 10 and name H3' )( resid 10 and name H1' ) 3.39 0.55 0.55 !384
assign ( resid 10 and name H1' )( resid 10 and name H4' ) 3.20 0.28 0.28 !343
assign ( resid 11 and name H8 )( resid 10 and name H2'' ) 2.30 0.63 0.63 !54
assign ( resid 11 and name H8 )( resid 10 and name H3' ) 3.97 0.89 0.89 !158
assign ( resid 11 and name H8 )( resid 10 and name H8 ) 4.26 1.01 1.01 !252
assign ( resid 11 and name H3' )( resid 11 and name H8 ) 3.58 0.59 0.59 !169
assign ( resid 11 and name H2'' )( resid 11 and name H1' ) 2.21 0.22 0.22 !290
assign ( resid 11 and name H3' )( resid 11 and name H1' ) 3.98 0.64 0.64 !360
assign ( resid 12 and name H6 )( resid 12 and name H1' ) 3.30 0.40 0.39 !212
assign ( resid 12 and name H6 )( resid 12 and name H4' ) 4.00 0.44 0.44 !108
assign (( resid 12 and name H5' ) or ( resid 12 and name H5'' ))
      ( resid 12 and name H6 ) 3.47 0.65 0.66 !83
!assign ( resid 12 and name H5 )( resid 12 and name H3' ) 2.91 0.65 0.65 !361
assign ( resid 12 and name H3' )( resid 12 and name H1' ) 3.11 1.00 1.00 !362
!assign (( resid 12 and name H5' ) or ( resid 12 and name H5'' ))
!      ( resid 12 and name H1' ) 2.54 0.34 0.35 !359
assign ( resid 12 and name H3' )( resid 12 and name H2'' ) 2.84 0.51 0.51 !418
assign (( resid 12 and name H5' ) or ( resid 12 and name H5'' ))
      ( resid 12 and name H3' ) 2.63 0.51 0.51 !444
assign (( resid 12 and name H5' ) or ( resid 12 and name H5'' ))
      ( resid 12 and name H4' ) 2.06 0.21 0.21 !449
assign ( resid 12 and name H6 )( resid 13 and name H5# ) 3.40 0.30 0.30 !4
assign ( resid 12 and name H5 )( resid 13 and name H5# ) 3.45 0.59 0.59 !272
!assign (( resid 12 and name H5' ) or ( resid 12 and name H5'' ))
!      ( resid 13 and name H5# ) 5.00 1.00 1.00 !404
assign ( resid 13 and name H6 )( resid 12 and name H1' ) 3.00 0.80 1.00 !229
assign ( resid 13 and name H6 )( resid 12 and name H3' ) 3.50 0.49 0.49 !168

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assign ( resid 13 and name H5# )( resid 12 and name H1' ) 5.14 0.53 0.53 !273
assign ( resid 13 and name H5# )( resid 12 and name H3' ) 2.61 0.30 0.50 !399
assign ( resid 13 and name H5# )( resid 12 and name H4' ) 4.71 1.29 1.29 !401
assign ( resid 14 and name H5# )( resid 13 and name H1' ) 4.16 0.50 0.50 !268
assign ( resid 14 and name H5# )( resid 13 and name H2' ) 2.90 0.48 0.48 !467
assign ( resid 14 and name H5# )( resid 13 and name H2'' ) 3.35 0.63 0.63 !468
assign ( resid 14 and name H6 )( resid 14 and name H5# ) 3.20 0.35 0.34 !44
assign ( resid 15 and name H5 )( resid 14 and name H5# ) 4.55 0.50 0.50 !275
assign ( resid 15 and name H5 )( resid 14 and name H1' ) 3.17 0.76 0.76 !387
assign ( resid 15 and name H5 )( resid 14 and name H2' ) 3.09 0.61 0.61 !292
assign ( resid 15 and name H5 )( resid 14 and name H3' ) 4.97 1.00 1.00 !378
assign ( resid 15 and name H5 )( resid 15 and name H2' ) 3.50 0.63 0.63 !282
assign ( resid 14 and name H2'' )( resid 15 and name H5 ) 2.87 0.41 0.41 !306
!assign ( resid 15 and name H5 )( resid 15 and name H3' ) 4.85 0.86 0.85 !377
assign ( resid 15 and name H5 )( resid 16 and name H5# ) 3.50 0.71 0.71 !274
assign ( resid 16 and name H5# )( resid 15 and name H1' ) 4.54 0.54 0.54 !271
assign ( resid 16 and name H6 )( resid 16 and name H1' ) 3.42 0.92 0.92 !227
assign ( resid 17 and name H5# )( resid 16 and name H1' ) 5.14 0.74 0.74 !276
assign ( resid 17 and name H6 )( resid 17 and name H1' ) 3.43 0.79 0.79 !195
assign ( resid 17 and name H3' )( resid 17 and name H1' ) 3.90 0.35 0.35 !373
assign ( resid 18 and name H8 )( resid 17 and name H2' ) 3.12 0.56 0.56 !11
assign ( resid 18 and name H8 )( resid 17 and name H3' ) 4.57 0.51 0.52 !153
assign ( resid 18 and name H3' )( resid 18 and name H8 ) 3.25 0.80 0.80 !154
assign ( resid 18 and name H8 )( resid 18 and name H4' ) 3.96 0.78 0.78 !102
assign ( resid 18 and name H3' )( resid 18 and name H1' ) 3.90 0.40 0.40 !372
assign ( resid 18 and name H1' )( resid 18 and name H4' ) 3.70 0.27 0.27 !341
assign ( resid 18 and name H4' )( resid 18 and name H2' ) 3.37 0.73 0.73 !423
assign ( resid 18 and name H8 )( resid 19 and name H5# ) 3.15 0.31 0.31 !1
!assign ( resid 18 and name H4' )( resid 19 and name H5# ) 5.70 1.24 1.23 !392
assign ( resid 19 and name H6 )( resid 18 and name H1' ) 3.10 0.43 0.43 !193
assign ( resid 19 and name H6 )( resid 18 and name H2'' ) 2.60 0.60 0.60 !52
assign ( resid 19 and name H5# )( resid 18 and name H1' ) 4.11 0.41 0.41 !266
assign ( resid 19 and name H5# )( resid 18 and name H2' ) 2.70 0.33 0.33 !465
assign ( resid 19 and name H5# )( resid 18 and name H2'' ) 3.67 0.44 0.45 !464
assign ( resid 19 and name H6 )( resid 19 and name H1' ) 3.14 0.59 0.59 !194
assign ( resid 19 and name H2' )( resid 19 and name H6 ) 2.34 0.34 0.35 !50
assign ( resid 19 and name H6 )( resid 19 and name H4' ) 4.11 0.73 0.72 !88
assign ( resid 19 and name H6 )( resid 19 and name H5# ) 2.34 0.50 0.50 !2
!assign ( resid 19 and name H2' )( resid 19 and name H5# ) 2.67 0.52 0.52 !466
assign ( resid 19 and name H2' )( resid 19 and name H1' ) 2.37 0.54 0.54 !289
assign ( resid 19 and name H3' )( resid 19 and name H1' ) 3.90 0.50 0.50 !369
assign ( resid 20 and name H6 )( resid 19 and name H6 ) 4.50 0.89 0.89 !260
assign ( resid 20 and name H5 )( resid 19 and name H6 ) 3.31 0.36 0.36 !192
assign ( resid 20 and name H5 )( resid 19 and name H5# ) 4.25 0.54 0.54 !267
assign ( resid 20 and name H5 )( resid 19 and name H1' ) 3.88 0.58 0.58 !388
assign ( resid 20 and name H5 )( resid 19 and name H2'' ) 2.96 0.39 0.38 !307

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assign ( resid 20 and name H4' )( resid 20 and name H2" ) 4.10 0.69 0.69 !420
!assign ( resid 21 and name H5 )( resid 20 and name H1' ) 3.63 0.59 0.59 !389
assign ( resid 21 and name H5 )( resid 20 and name H2' ) 3.44 0.46 0.46 !285
!assign ( resid 21 and name H5 )( resid 20 and name H3' ) 3.40 0.68 0.68 !374
assign ( resid 21 and name H2' )( resid 21 and name H6 ) 2.09 0.21 0.21 !49
assign ( resid 21 and name H5 )( resid 21 and name H2' ) 3.50 0.78 0.78 !280
assign ( resid 21 and name H2' )( resid 21 and name H1' ) 2.29 1.00 1.00 !281
assign ( resid 21 and name H2" )( resid 21 and name H1' ) 2.04 0.20 0.20 !294
assign ( resid 21 and name H3' )( resid 21 and name H1' ) 3.90 0.48 0.48 !377
assign ( resid 21 and name H3' )( resid 21 and name H2' ) 2.26 0.23 0.23 !406
!assign ( resid 21 and name H4' )( resid 21 and name H2' ) 2.62 0.62 0.62 !407
assign ( resid 22 and name H8 )( resid 21 and name H1' ) 2.98 0.60 0.60 !209
assign ( resid 22 and name H8 )( resid 21 and name H2' ) 2.91 0.49 0.49 !7
assign ( resid 22 and name H8 )( resid 21 and name H3' ) 4.05 0.67 0.68 !150
assign ( resid 22 and name H8 )( resid 21 and name H6 ) 3.83 1.02 1.02 !253
assign ( resid 22 and name H8 )( resid 22 and name H1' ) 3.29 0.73 0.73 !223
assign ( resid 22 and name H3' )( resid 22 and name H8 ) 3.72 0.44 0.45 !147
assign ( resid 22 and name H8 )( resid 22 and name H4' ) 4.19 0.80 0.79 !113
assign ( resid 22 and name H3' )( resid 22 and name H1' ) 3.25 0.88 0.88 !365
assign ( resid 22 and name H3' )( resid 22 and name H2' ) 2.29 0.23 0.23 !417
assign ( resid 22 and name H4' )( resid 22 and name H2" ) 3.50 0.85 0.85 !419
!Added restrains
assign ( resid 6 and name HA )( resid 16 and name H5# ) 4.50 0.70 0.70
assign ( resid 6 and name HB" )( resid 16 and name H5# ) 6.00 0.80 0.80
!Water restrains
assign ( resid 6 and name HB' )( resid 17 and name H3 ) 4.00 1.00 1.00
assign ( resid 6 and name HB' )( resid 18 and name H1 ) 4.50 1.00 1.00
assign ( resid 6 and name HB" )( resid 17 and name H3 ) 5.00 1.00 1.00
assign ( resid 6 and name HB" )( resid 18 and name H1 ) 5.50 1.00 1.00
assign ( resid 6 and name HA )( resid 17 and name H3 ) 5.00 0.50 0.50
assign ( resid 6 and name H6 )( resid 6 and name HB' ) 2.50 1.00 1.00
assign ( resid 6 and name H6 )( resid 6 and name HA ) 2.50 1.00 1.00
assign ( resid 5 and name H4# )( resid 6 and name HB' ) 4.50 1.00 1.00
assign ( resid 6 and name HOA )( resid 6 and name HA ) 2.50 1.00 1.00
assign ( resid 6 and name HOA )( resid 6 and name HB' ) 3.50 1.00 1.00
assign ( resid 6 and name HOA )( resid 7 and name H6# ) 4.50 1.00 1.00
assign ( resid 6 and name HOA )( resid 16 and name H5# ) 3.50 1.00 1.00
assign ( resid 6 and name HOA )( resid 6 and name HB" ) 4.00 1.00 1.00
assign ( resid 6 and name HOA )( resid 6 and name H6 ) 4.00 1.00 1.00
!Water theoretical restrains
assign ( resid 11 and name H1 )( resid 13 and name H3 ) 3.38 0.20 0.20
assign ( resid 13 and name H3 )( resid 14 and name H3 ) 3.49 0.10 0.10
assign ( resid 14 and name H3 )( resid 8 and name H1 ) 3.73 0.10 0.10
assign ( resid 8 and name H1 )( resid 16 and name H3 ) 3.18 0.10 0.10
assign ( resid 16 and name H3 )( resid 17 and name H3 ) 3.49 0.10 0.10
assign ( resid 17 and name H3 )( resid 18 and name H1 ) 4.13 0.10 0.10

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assign ( resid 18 and name H1 )( resid 19 and name H3 ) 3.49 0.10 0.10
assign ( resid 19 and name H3 )( resid 3 and name H1 ) 3.73 0.10 0.10
assign ( resid 3 and name H1 )( resid 2 and name H1 ) 3.41 0.10 0.10
assign ( resid 2 and name H1 )( resid 22 and name H1 ) 3.71 0.20 0.20
!More Water theoretical restrains
assign ( resid 21 and name H41 )( resid 3 and name H1 ) 3.88 0.10 0.10
assign ( resid 20 and name H41 )( resid 2 and name H1 ) 4.43 0.10 0.10
assign ( resid 20 and name H41 )( resid 19 and name H3 ) 3.60 0.10 0.10
assign ( resid 18 and name H1 )( resid 6 and name H2 ) 3.96 0.10 0.10
assign ( resid 18 and name H1 )( resid 4 and name H2 ) 3.81 0.10 0.10
assign ( resid 17 and name H3 )( resid 7 and name H2 ) 3.92 0.10 0.10
assign ( resid 7 and name H2 )( resid 8 and name H1 ) 4.32 0.10 0.10
assign ( resid 8 and name H1 )( resid 9 and name H2 ) 3.92 0.10 0.10
assign ( resid 9 and name H61 )( resid 13 and name H3 ) 3.92 0.10 0.10
assign ( resid 14 and name H3 )( resid 15 and name H41 ) 3.60 0.10 0.10
assign ( resid 16 and name H3 )( resid 15 and name H41 ) 4.49 0.10 0.10

set message=on echo=on end

set message=off echo=off end
assign ( resid 1 and name H6 )( resid 1 and name H1' ) 3.70 0.48 0.48 !199
assign ( resid 1 and name H2' )( resid 1 and name H6 ) 2.11 0.21 0.21 !48
!assign ( resid 1 and name H5 )( resid 1 and name H1' ) 5.00 0.81 0.81 !390
assign ( resid 1 and name H2'' )( resid 1 and name H1' ) 2.02 0.20 0.20 !295
assign ( resid 1 and name H1' )( resid 1 and name H4' ) 3.70 0.46 0.46 !333
assign ( resid 2 and name H8 )( resid 1 and name H3' ) 3.45 0.56 0.55 !146
assign ( resid 2 and name H3' )( resid 2 and name H1' ) 3.45 0.50 0.50 !380
assign (( resid 2 and name H5' ) or ( resid 2 and name H5'' ))
      ( resid 2 and name H3' ) 3.31 0.58 0.58 !447
assign (( resid 2 and name H5' ) or ( resid 2 and name H5'' ))
      ( resid 2 and name H4' ) 2.19 0.28 0.28 !448
assign ( resid 3 and name H5' )( resid 3 and name H8 ) 3.25 0.71 0.71 !105
assign ( resid 4 and name H8 )( resid 3 and name H1' ) 2.58 0.28 0.27 !208
assign ( resid 4 and name H8 )( resid 4 and name H4' ) 4.00 0.80 0.80 !117
assign (( resid 4 and name H5' ) or ( resid 4 and name H5'' ))
      ( resid 4 and name H8 ) 4.33 0.92 0.92 !124
assign ( resid 4 and name H1' )( resid 4 and name H4' ) 3.70 0.31 0.31 !345
assign ( resid 4 and name H4' )( resid 4 and name H2'' ) 3.73 0.59 0.59 !428
assign (( resid 4 and name H5' ) or ( resid 4 and name H5'' ))
      ( resid 3 and name H2'' ) 3.05 0.41 0.41 !441
assign ( resid 5 and name H3' )( resid 5 and name H2'' ) 2.50 0.29 0.28 !410
assign ( resid 6 and name H8 )( resid 6 and name H1' ) 3.10 0.76 0.76 !206
assign ( resid 6 and name H3' )( resid 6 and name H8 ) 3.50 0.80 0.80 !161
assign ( resid 6 and name H3' )( resid 6 and name H4' ) 2.43 0.24 0.24 !460
assign ( resid 6 and name H2 )( resid 7 and name H2 ) 3.40 0.34 0.34 !258
assign ( resid 7 and name H1' )( resid 7 and name H4' ) 3.16 0.50 0.50 !344

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assign ( resid 8 and name H8 )( resid 8 and name H1' ) 3.25 0.97 0.96 !159
assign ( resid 8 and name H2' )( resid 8 and name H1' ) 2.71 0.38 0.39 !304
assign ( resid 8 and name H2" )( resid 8 and name H1' ) 2.17 0.23 0.23 !305
assign ( resid 9 and name H8 )( resid 9 and name H1' ) 3.00 0.85 0.85 !219
assign ( resid 9 and name H2 )( resid 10 and name H2 ) 3.65 0.36 0.36 !259
assign ( resid 9 and name H2 )( resid 15 and name H1' ) 3.28 0.33 0.33 !191
assign ( resid 10 and name H8 )( resid 9 and name H1' ) 2.81 0.38 0.38 !218
assign ( resid 10 and name H8 )( resid 10 and name H4' ) 4.00 0.97 0.97 !115
assign (( resid 10 and name H5' ) or ( resid 10 and name H5" ))
      ( resid 10 and name H8 ) 4.16 0.92 0.92 !122
assign (( resid 10 and name H5' ) or ( resid 10 and name H5" ))
      ( resid 9 and name H2" ) 2.99 0.30 0.30 !442
assign ( resid 11 and name H3' )( resid 11 and name H2" ) 2.78 0.54 0.54 !411
assign (( resid 11 and name H5' ) or ( resid 11 and name H5" ))
      ( resid 11 and name H3' ) 3.12 0.35 0.35 !453
assign ( resid 12 and name H2" )( resid 12 and name H6 ) 3.10 0.62 0.62 !28
assign ( resid 12 and name H3' )( resid 12 and name H6 ) 3.00 0.80 0.80 !145
assign ( resid 12 and name H1' )( resid 12 and name H4' ) 3.60 0.33 0.33 !331
assign ( resid 12 and name H1' )( resid 13 and name H4' ) 4.20 0.33 0.33 !331
assign ( resid 13 and name H5# )( resid 12 and name H2' ) 3.25 0.90 0.67 !475
assign ( resid 13 and name H6 )( resid 13 and name H1' ) 3.70 0.64 0.64 !224
assign ( resid 13 and name H3' )( resid 13 and name H6 ) 3.50 0.80 0.80 !173
assign ( resid 13 and name H6 )( resid 13 and name H4' ) 3.71 0.80 0.80 !98
assign ( resid 13 and name H6 )( resid 14 and name H5# ) 3.07 0.60 0.60 !3
assign ( resid 14 and name H6 )( resid 13 and name H1' ) 2.70 0.74 0.74 !237
!assign ( resid 14 and name H6 )( resid 13 and name H6 ) 2.85 0.60 0.60 !262
assign ( resid 14 and name H5# )( resid 13 and name H3' ) 4.07 0.59 0.59 !393
assign ( resid 14 and name H6 )( resid 14 and name H4' ) 4.60 0.67 0.67 !91
assign ( resid 15 and name H6 )( resid 14 and name H3' ) 4.00 0.80 0.80 !172
assign ( resid 15 and name H5 )( resid 14 and name H6 ) 3.42 0.50 0.50 !196
!assign ( resid 15 and name H6 )( resid 14 and name H5# ) 4.74 0.47 0.47 !41
assign ( resid 15 and name H6 )( resid 15 and name H1' ) 3.70 0.48 0.48 !228
assign ( resid 15 and name H3' )( resid 15 and name H6 ) 3.50 0.80 0.80 !171
assign ( resid 15 and name H2' )( resid 15 and name H1' ) 2.63 0.37 0.37 !287
assign ( resid 15 and name H3' )( resid 15 and name H1' ) 3.13 0.80 0.80 !370
assign ( resid 15 and name H6 )( resid 16 and name H5# ) 3.00 0.80 0.80 !42
assign ( resid 16 and name H5# )( resid 15 and name H2' ) 2.99 0.30 0.30 !477
assign ( resid 16 and name H5# )( resid 15 and name H3' ) 4.01 0.89 0.89 !395
assign ( resid 16 and name H2" )( resid 16 and name H6 ) 3.40 0.49 0.48 !55
assign ( resid 16 and name H6 )( resid 16 and name H5# ) 2.33 1.00 1.00 !43
assign (( resid 6 and name HS5 ) or ( resid 6 and name HS4 ))
      ( resid 16 and name H5# ) 3.46 0.53 0.54 !45
assign ( resid 17 and name H5# )( resid 16 and name H2" ) 3.73 0.48 0.48 !471
assign ( resid 17 and name H5# )( resid 16 and name H3' ) 4.81 0.95 0.95 !396
assign ( resid 17 and name H6 )( resid 17 and name H5# ) 3.20 0.26 0.25 !46
assign ( resid 18 and name H8 )( resid 17 and name H1' ) 2.78 0.48 0.48 !214

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!assign ( resid 18 and name H8 )( resid 17 and name H6 ) 4.80 0.65 0.65 !256
assign ( resid 18 and name H8 )( resid 18 and name H1' ) 3.20 0.58 0.57 !215
assign ( resid 18 and name H2' )( resid 18 and name H8 ) 2.24 0.22 0.22 !12
assign ( resid 18 and name H5' )( resid 18 and name H8 ) 3.15 0.75 0.75 !107
assign ( resid 18 and name H2' )( resid 18 and name H1' ) 2.46 0.40 0.40 !313
assign ( resid 18 and name H2'' )( resid 18 and name H1' ) 2.20 0.22 0.22 !315
assign ( resid 18 and name H3' )( resid 18 and name H4' ) 2.49 0.25 0.25 !457
!assign ( resid 19 and name H6 )( resid 18 and name H8 ) 3.43 0.99 1.00 !257
assign ( resid 19 and name H5# )( resid 18 and name H3' ) 3.90 0.36 0.36 !391
assign ( resid 19 and name H3' )( resid 19 and name H6 ) 3.00 0.80 0.80 !183
!assign ( resid 20 and name H5 )( resid 19 and name H3' ) 3.75 0.85 0.86 !376
assign ( resid 20 and name H2' )( resid 20 and name H1' ) 2.33 0.60 0.60 !286
assign ( resid 20 and name H3' )( resid 20 and name H1' ) 3.27 0.65 0.65 !371
assign ( resid 21 and name H6 )( resid 20 and name H1' ) 3.92 0.75 0.75 !232
assign ( resid 21 and name H6 )( resid 20 and name H2'' ) 2.83 0.38 0.38 !64
assign ( resid 21 and name H6 )( resid 21 and name H1' ) 3.30 0.52 0.53 !197
assign ( resid 21 and name H3' )( resid 21 and name H2'' ) 2.50 0.32 0.33 !415
assign ( resid 22 and name H2' )( resid 22 and name H8 ) 2.19 0.22 0.22 !26
assign ( resid 22 and name H2'' )( resid 22 and name H1' ) 2.06 0.21 0.21 !300
assign ( resid 22 and name H3' )( resid 22 and name H4' ) 2.60 0.22 0.22 !456

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set message=on echo=on end

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set message=off echo=off end
assign ( resid 2 and name H8 )( resid 1 and name H2'' ) 2.72 0.37 0.37 !10
assign ( resid 2 and name H2' )( resid 2 and name H1' ) 2.77 0.58 0.58 !308
assign ( resid 2 and name H2'' )( resid 2 and name H1' ) 2.30 0.20 0.20 !309
assign ( resid 2 and name H3' )( resid 2 and name H4' ) 2.60 0.24 0.23 !461
assign ( resid 3 and name H2'' )( resid 3 and name H8 ) 3.70 0.46 0.46 !32
assign ( resid 3 and name H2'' )( resid 3 and name H1' ) 2.28 0.32 0.32 !312
assign ( resid 3 and name H4' )( resid 3 and name H2'' ) 4.10 0.49 0.50 !431
assign ( resid 4 and name H8 )( resid 3 and name H2' ) 2.93 0.44 0.44 !21
assign ( resid 4 and name H2' )( resid 4 and name H8 ) 2.25 0.27 0.26 !22
assign ( resid 4 and name H4' )( resid 4 and name H2' ) 3.80 0.30 0.30 !425
assign ( resid 6 and name H2' )( resid 6 and name H8 ) 2.11 0.22 0.23 !13
assign ( resid 6 and name H2'' )( resid 6 and name H8 ) 3.40 0.43 0.42 !14
assign ( resid 6 and name H5' )( resid 6 and name H8 ) 3.49 0.84 0.83 !127
assign ( resid 6 and name H5'' )( resid 6 and name H8 ) 3.96 0.65 0.65 !129
assign ( resid 6 and name HA )( resid 6 and name HS1 )
or ( resid 6 and name HS5 ) 2.27 0.28 0.29 !178
assign ( resid 7 and name H8 )( resid 6 and name H1' ) 2.69 0.52 0.52 !207
assign ( resid 7 and name H3' )( resid 7 and name H8 ) 3.50 0.80 0.80 !162
assign ( resid 7 and name H3' )( resid 7 and name H4' ) 2.38 0.40 0.40 !458
assign ( resid 8 and name H8 )( resid 7 and name H1' ) 3.15 0.60 0.60 !225
assign ( resid 8 and name H2' )( resid 8 and name H8 ) 2.25 0.31 0.31 !69
assign ( resid 8 and name H8 )( resid 8 and name H4' ) 4.90 0.52 0.53 !99

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assign ( resid 9 and name H8 )( resid 8 and name H3' ) 4.50 0.79 0.79 !164
assign ( resid 9 and name H8 )( resid 9 and name H4' ) 4.50 0.52 0.52 !116
assign (( resid 9 and name H5' ) or ( resid 9 and name H5" ))
      ( resid 9 and name H8 ) 3.77 0.65 0.65 !123
assign ( resid 9 and name H2 )( resid 10 and name H1' ) 4.04 0.40 0.40 !190
assign ( resid 10 and name H2 )( resid 10 and name H1' ) 4.11 0.41 0.41 !243
assign ( resid 10 and name H4' )( resid 10 and name H2' ) 3.16 0.70 0.70 !424
assign ( resid 10 and name H4' )( resid 10 and name H2" ) 4.10 0.50 0.50 !429
assign ( resid 9 and name H4' )( resid 9 and name H2" ) 4.10 0.50 0.50 !429
assign ( resid 10 and name H3' )( resid 10 and name H4' ) 2.60 0.18 0.18 !459
assign ( resid 4 and name H3' )( resid 4 and name H4' ) 2.60 0.18 0.18 !459
assign ( resid 10 and name H2 )( resid 11 and name H1' ) 4.57 0.46 0.46 !242
assign ( resid 11 and name H8 )( resid 10 and name H1' ) 2.88 0.35 0.35 !236
assign (( resid 11 and name H5' ) or ( resid 11 and name H5" ))
      ( resid 11 and name H8 ) 4.28 0.73 0.73 !95
assign ( resid 11 and name H2' )( resid 11 and name H1' ) 2.60 0.40 0.40 !297
assign ( resid 11 and name H3' )( resid 11 and name H2' ) 2.23 0.22 0.22 !412
assign ( resid 11 and name H3' )( resid 11 and name H4' ) 2.31 0.40 0.40 !454
assign ( resid 12 and name H2' )( resid 12 and name H6 ) 2.77 0.52 0.52 !29
assign ( resid 12 and name H2' )( resid 12 and name H1' ) 3.00 0.28 0.28 !296
assign ( resid 12 and name H3' )( resid 12 and name H4' ) 2.60 0.21 0.21 !462
assign ( resid 13 and name H6 )( resid 12 and name H2' ) 2.27 0.32 0.33 !36
assign ( resid 13 and name H5# )( resid 12 and name H2" ) 3.38 0.48 0.48 !470
assign ( resid 13 and name H6 )( resid 13 and name H5# ) 3.20 0.33 0.33 !40
assign ( resid 13 and name H2' )( resid 13 and name H5# ) 4.60 0.85 0.85 !476
assign ( resid 13 and name H3' )( resid 13 and name H1' ) 3.90 0.50 0.50 !366
assign ( resid 14 and name H3' )( resid 13 and name H1' ) 4.50 0.50 0.50 !366
assign ( resid 14 and name H5' )( resid 14 and name H6 ) 2.93 0.53 0.53 !92
assign ( resid 15 and name H6 )( resid 14 and name H1' ) 2.70 0.45 0.45 !226
assign ( resid 15 and name H3' )( resid 15 and name H2' ) 2.50 0.19 0.19 !409
assign ( resid 20 and name H3' )( resid 20 and name H2' ) 2.50 0.19 0.19 !409
assign ( resid 16 and name H6 )( resid 15 and name H1' ) 3.07 0.70 0.70 !235
assign ( resid 16 and name H5# )( resid 15 and name H2" ) 3.68 0.61 0.62 !469
assign ( resid 16 and name H3' )( resid 16 and name H6 ) 3.50 0.80 0.80 !176
assign ( resid 16 and name H6 )( resid 16 and name H4' ) 3.90 0.80 0.80 !94
!assign ( resid 16 and name H3' )( resid 16 and name H5# ) 4.19 0.60 0.60 !394
assign ( resid 16 and name H2' )( resid 16 and name H1' ) 2.58 0.47 0.48 !288
assign ( resid 16 and name H3' )( resid 16 and name H1' ) 3.60 0.52 0.51 !368
!assign ( resid 17 and name H3' )( resid 16 and name H1' ) 4.50 0.52 0.51 !368
assign ( resid 16 and name H6 )( resid 17 and name H5# ) 3.04 0.36 0.36 !47
assign ( resid 17 and name H6 )( resid 16 and name H1' ) 3.05 0.71 0.72 !233
assign ( resid 17 and name H6 )( resid 16 and name H2" ) 2.57 0.38 0.38 !57
assign ( resid 17 and name H2' )( resid 17 and name H1' ) 2.73 0.52 0.52 !291
assign ( resid 18 and name H5" )( resid 18 and name H8 ) 4.50 0.44 0.44 !106
assign ( resid 18 and name H3' )( resid 18 and name H2" ) 2.77 0.33 0.33 !435
assign ( resid 18 and name H4' )( resid 18 and name H2" ) 4.00 0.28 0.28 !440

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assign ( resid 6 and name H4' )( resid 6 and name H2" ) 4.00 0.28 0.28 !440
assign ( resid 20 and name H6 )( resid 19 and name H1' ) 3.34 0.62 0.62 !245
assign ( resid 20 and name H6 )( resid 19 and name H3' ) 3.65 0.79 0.79 !174
assign ( resid 20 and name H5 )( resid 19 and name H2' ) 3.02 0.56 0.56 !284
assign ( resid 20 and name H2" )( resid 20 and name H6 ) 3.40 0.33 0.33 !67
assign ( resid 20 and name H3' )( resid 20 and name H6 ) 3.50 0.80 0.80 !175
assign ( resid 20 and name H5 )( resid 20 and name H2' ) 4.30 0.49 0.49 !283
assign ( resid 20 and name H2" )( resid 20 and name H1' ) 2.19 0.26 0.25 !301
assign ( resid 20 and name H3' )( resid 20 and name H2" ) 2.49 0.25 0.25 !416
assign ( resid 21 and name H5 )( resid 20 and name H2" ) 3.08 0.40 0.40 !302
assign ( resid 21 and name H1' )( resid 21 and name H4' ) 3.00 0.35 0.35 !334
assign ( resid 22 and name H5' )( resid 21 and name H2" ) 2.38 0.29 0.30 !421
assign (( resid 22 and name H5' ) or ( resid 22 and name H5" ))
      ( resid 22 and name H8 ) 4.39 0.68 0.68 !111
assign ( resid 22 and name H3' )( resid 22 and name H2" ) 2.46 0.40 0.40 !413

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set message=on echo=on end

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set message=off echo=off end
assign ( resid 1 and name H4' )( resid 1 and name H2" ) 4.10 0.43 0.43 !422
assign ( resid 1 and name H3' )( resid 1 and name H4' ) 2.60 0.19 0.19 !455
assign ( resid 3 and name H5" )( resid 3 and name H8 ) 3.98 0.94 0.94 !137
assign ( resid 3 and name H2' )( resid 3 and name H1' ) 3.00 0.39 0.38 !310
assign ( resid 3 and name H3' )( resid 3 and name H1' ) 3.33 0.60 0.60 !382
assign ( resid 4 and name H5' )( resid 3 and name H1' ) 2.53 0.31 0.30 !353
assign ( resid 4 and name H8 )( resid 3 and name H3' ) 4.04 0.54 0.54 !167
assign ( resid 4 and name H3' )( resid 4 and name H8 ) 4.40 0.61 0.61 !163
assign ( resid 5 and name H1' )( resid 5 and name H4' ) 3.50 0.27 0.27 !335
assign ( resid 5 and name H3' )( resid 5 and name H4' ) 2.60 0.20 0.20 !463
!assign ( resid 6 and name H8 )( resid 5 and name H4' ) 3.62 0.67 0.67 !128
assign ( resid 6 and name H3' )( resid 6 and name H1' ) 3.32 0.60 0.60 !382
assign ( resid 6 and name H4' )( resid 6 and name H2' ) 3.38 0.53 0.53 !439
assign ( resid 7 and name H8 )( resid 6 and name H2" ) 2.30 0.26 0.26 !16
assign ( resid 7 and name H8 )( resid 6 and name H3' ) 3.94 0.73 0.73 !182
assign ( resid 7 and name H2 )( resid 7 and name H1' ) 4.50 0.33 0.33 !240
assign ( resid 7 and name H2' )( resid 7 and name H1' ) 3.00 0.22 0.22 !323
assign ( resid 7 and name H5" )( resid 7 and name H4' ) 2.12 0.30 0.31 !451
assign ( resid 7 and name H2 )( resid 8 and name H1' ) 4.48 0.61 0.62 !184
assign ( resid 8 and name H8 )( resid 7 and name H2' ) 2.73 0.31 0.31 !70
assign ( resid 9 and name H2" )( resid 9 and name H8 ) 3.70 0.52 0.51 !19
assign ( resid 9 and name H3' )( resid 9 and name H8 ) 4.40 0.50 0.50 !165
assign ( resid 9 and name H2' )( resid 9 and name H1' ) 2.48 0.42 0.42 !316
assign ( resid 11 and name H8 )( resid 10 and name H2' ) 3.00 0.50 0.50 !76
assign ( resid 11 and name H8 )( resid 11 and name H1' ) 3.50 0.48 0.48 !244
assign ( resid 11 and name H8 )( resid 11 and name H4' ) 4.90 0.53 0.53 !134
assign ( resid 13 and name H2' )( resid 13 and name H6 ) 2.43 0.42 0.42 !37

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assign ( resid 13 and name H2' )( resid 13 and name H1' ) 3.00 0.31 0.31 !299
!assign ( resid 14 and name H2' )( resid 13 and name H1' ) 4.10 0.31 0.31 !299
assign ( resid 13 and name H2'' )( resid 13 and name H1' ) 2.16 0.22 0.22 !326
assign ( resid 13 and name H1' )( resid 13 and name H4' ) 3.70 0.44 0.44 !346
assign ( resid 14 and name H6 )( resid 14 and name H1' ) 3.00 0.62 0.62 !239
assign ( resid 14 and name H2' )( resid 14 and name H1' ) 3.02 0.63 0.63 !298
assign ( resid 14 and name H3' )( resid 14 and name H1' ) 3.90 0.54 0.54 !367
assign ( resid 14 and name H3' )( resid 14 and name H2' ) 2.00 0.20 0.20 !414
assign ( resid 15 and name H6 )( resid 14 and name H2' ) 2.77 0.58 0.58 !38
assign ( resid 15 and name H2' )( resid 15 and name H6 ) 2.37 0.35 0.35 !39
assign ( resid 15 and name H2'' )( resid 15 and name H1' ) 2.30 0.19 0.19 !317
assign ( resid 17 and name H6 )( resid 16 and name H2' ) 3.00 0.31 0.60 !59
assign ( resid 17 and name H6 )( resid 17 and name H4' ) 4.60 0.45 0.44 !130
assign ( resid 17 and name H1' )( resid 17 and name H4' ) 3.70 0.50 0.50 !332
assign ( resid 18 and name H8 )( resid 17 and name H2'' ) 2.50 0.33 0.32 !30
assign ( resid 18 and name H2'' )( resid 18 and name H8 ) 3.70 0.27 0.27 !31
assign ( resid 19 and name H6 )( resid 18 and name H3' ) 4.00 0.81 0.81 !181
assign ( resid 19 and name H2'' )( resid 19 and name H1' ) 2.14 0.21 0.21 !318
!assign ( resid 19 and name H1' )( resid 19 and name H4' ) 2.30 0.27 0.28 !350
assign ( resid 20 and name H6 )( resid 20 and name H1' ) 3.12 0.64 0.63 !234
assign ( resid 21 and name H2'' )( resid 21 and name H6 ) 3.40 0.33 0.33 !63
assign (( resid 22 and name H5' ) or ( resid 22 and name H5'' ))
      ( resid 21 and name H1' ) 3.67 0.47 0.47 !355
!assign ( resid 22 and name H8 )( resid 21 and name H4' ) 3.57 1.08 1.08 !112

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set message=on echo=on end

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set message=off echo=off end
assign ( resid 1 and name H2'' )( resid 1 and name H6 ) 3.40 0.28 0.28 !68
assign ( resid 1 and name H6 )( resid 1 and name H4' ) 3.66 0.68 0.68 !93
assign ( resid 2 and name H2' )( resid 2 and name H8 ) 2.20 0.27 0.26 !27
assign ( resid 2 and name H2'' )( resid 2 and name H8 ) 3.70 0.37 0.37 !27
assign ( resid 3 and name H8 )( resid 2 and name H2' ) 3.46 0.73 0.72 !33
assign ( resid 3 and name H8 )( resid 2 and name H2'' ) 2.67 0.36 0.36 !33
assign ( resid 3 and name H8 )( resid 2 and name H8 ) 4.24 0.69 0.69 !264
assign ( resid 3 and name H2' )( resid 3 and name H8 ) 2.22 0.33 0.33 !33
assign ( resid 4 and name H8 )( resid 3 and name H2'' ) 2.10 0.41 0.41 !18
assign ( resid 4 and name H2'' )( resid 4 and name H8 ) 3.70 0.35 0.35 !18
assign ( resid 4 and name H2' )( resid 4 and name H1' ) 3.00 0.21 0.21 !328
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS5' ) or
      ( resid 6 and name HS2 ) or ( resid 6 and name HS4 ))
      ( resid 5 and name H5 ) 4.89 0.49 0.49 !179
assign ( resid 6 and name H2' )( resid 6 and name H1' ) 2.66 0.54 0.54 !329
assign ( resid 6 and name H2'' )( resid 6 and name H1' ) 2.05 0.26 0.26 !311
assign ( resid 7 and name H8 )( resid 6 and name H2' ) 2.95 0.75 0.75 !15
assign ( resid 7 and name H2' )( resid 7 and name H8 ) 2.29 0.27 0.27 !15

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assign ( resid 7 and name H5' )( resid 7 and name H4' ) 2.50 0.19 0.19 !452
assign ( resid 8 and name H2'' )( resid 8 and name H8 ) 3.70 0.27 0.27 !73
assign ( resid 8 and name H5' )( resid 8 and name H8 ) 3.48 0.62 0.62 !101
assign ( resid 9 and name H8 ) ( resid 8 and name H2' ) 3.00 0.42 0.42 !25
assign ( resid 9 and name H2' )( resid 9 and name H8 ) 2.20 0.21 0.22 !23
assign ( resid 10 and name H8 ) ( resid 9 and name H2' ) 2.67 0.42 0.42 !24
assign ( resid 10 and name H8 ) ( resid 9 and name H2'' ) 2.30 0.48 0.48 !20
assign ( resid 10 and name H8 ) ( resid 9 and name H3' ) 4.90 0.52 0.52 !166
assign ( resid 10 and name H2' )( resid 10 and name H8 ) 2.29 0.32 0.32 !24
assign ( resid 10 and name H2'' )( resid 10 and name H8 ) 3.70 0.41 0.40 !20
assign ( resid 10 and name H3' )( resid 10 and name H8 ) 4.40 0.58 0.58 !166
assign ( resid 10 and name H2' )( resid 10 and name H1' ) 2.48 0.56 0.56 !330
assign ( resid 11 and name H2' )( resid 11 and name H8 ) 2.39 0.25 0.25 !68
assign ( resid 11 and name H2'' )( resid 11 and name H8 ) 3.70 0.62 0.62 !60
!assign ( resid 11 and name H1' )( resid 11 and name H4' ) 2.58 0.27 0.27 !348
assign ( resid 12 and name H2'' )( resid 12 and name H1' ) 2.05 0.21 0.21 !314
assign ( resid 13 and name H6 ) ( resid 12 and name H2'' ) 2.10 0.58 0.57 !35
!assign ( resid 13 and name H6 ) ( resid 12 and name H4' ) 3.98 0.88 0.88 !97
assign ( resid 13 and name H2'' )( resid 13 and name H6 ) 3.40 0.37 0.36 !35
assign ( resid 13 and name H5' )( resid 13 and name H6 ) 3.66 0.62 0.62 !97
assign ( resid 14 and name H6 ) ( resid 13 and name H2'' ) 2.62 0.61 0.61 !77
assign ( resid 14 and name H6 ) ( resid 13 and name H3' ) 4.80 0.67 0.67 !180
assign ( resid 14 and name H2' )( resid 14 and name H6 ) 2.39 0.49 0.49 !58
assign ( resid 14 and name H2'' )( resid 14 and name H6 ) 3.02 0.65 0.65 !56
assign ( resid 14 and name H3' )( resid 14 and name H6 ) 4.00 0.46 0.46 !180
assign ( resid 14 and name H2'' )( resid 14 and name H1' ) 2.04 0.21 0.21 !327
!assign ( resid 14 and name H1' )( resid 14 and name H4' ) 2.23 0.24 0.23 !351
assign ( resid 14 and name H3' )( resid 14 and name H2'' ) 2.70 0.33 0.32 !437
assign ( resid 15 and name H6 ) ( resid 14 and name H2'' ) 2.30 0.48 0.47 !74
assign ( resid 15 and name H2'' )( resid 15 and name H6 ) 3.40 0.43 0.43 !75
!assign ( resid 15 and name H6 ) ( resid 15 and name H4' ) 2.69 0.39 0.39 !101
!assign ( resid 15 and name H1' )( resid 15 and name H4' ) 2.44 0.27 0.27 !349
assign ( resid 16 and name H6 ) ( resid 15 and name H2' ) 3.02 0.69 0.69 !32
assign ( resid 16 and name H6 ) ( resid 15 and name H2'' ) 2.73 0.52 0.52 !66
assign ( resid 16 and name H6 ) ( resid 15 and name H3' ) 4.80 0.52 0.52 !177
assign ( resid 16 and name H2' )( resid 16 and name H6 ) 2.07 0.23 0.23 !62
assign ( resid 16 and name H2'' )( resid 16 and name H1' ) 2.30 0.19 0.19 !324
assign ( resid 16 and name H3' )( resid 16 and name H2' ) 2.06 0.24 0.25 !436
assign ( resid 16 and name H3' )( resid 16 and name H2'' ) 2.45 0.44 0.44 !438
assign ( resid 17 and name H6 ) ( resid 16 and name H3' ) 4.80 0.66 0.65 !180
assign ( resid 17 and name H2' )( resid 17 and name H6 ) 2.02 0.23 0.23 !58
assign ( resid 17 and name H2'' )( resid 17 and name H6 ) 2.96 0.66 0.65 !56
assign ( resid 17 and name H3' )( resid 17 and name H6 ) 3.38 0.80 0.80 !180
assign ( resid 17 and name H2'' )( resid 17 and name H1' ) 2.06 0.21 0.21 !314
assign ( resid 19 and name H6 ) ( resid 18 and name H2' ) 2.60 0.41 0.41 !51
assign ( resid 19 and name H2'' )( resid 19 and name H6 ) 3.50 0.60 0.60 !51

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15

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!assign (( resid 19 and name H5' ) or ( resid 19 and name H5" ))
!
      ( resid 19 and name H1' ) 3.31 0.50 0.50 !354
assign ( resid 20 and name H6 )( resid 19 and name H2' ) 2.54 0.33 0.33 !61
assign ( resid 20 and name H6 )( resid 19 and name H2" ) 2.10 0.46 0.45 !65
assign ( resid 20 and name H2' )( resid 20 and name H6 ) 2.25 0.26 0.25 !61
assign ( resid 20 and name H6 )( resid 20 and name H5' ) 3.69 0.90 0.90 !93
assign ( resid 20 and name H5' )( resid 20 and name H6 ) 3.30 0.54 0.55 !133
!assign ( resid 20 and name H1' )( resid 20 and name H4' ) 2.16 0.25 0.25 !347
assign ( resid 21 and name H6 )( resid 20 and name H2' ) 3.14 0.64 0.64 !62
assign ( resid 21 and name H6 )( resid 20 and name H3' ) 4.80 0.43 0.42 !177
assign ( resid 21 and name H3' )( resid 21 and name H6 ) 3.50 0.80 0.80 !177
assign ( resid 21 and name H6 )( resid 21 and name H4' ) 4.60 0.55 0.56 !131
assign ( resid 21 and name H5' )( resid 21 and name H6 ) 3.50 0.65 0.66 !135
assign ( resid 21 and name H3' )( resid 21 and name H1' ) 3.07 0.88 0.88 !377
assign ( resid 22 and name H8 )( resid 21 and name H2" ) 2.30 0.46 0.46 !9
assign ( resid 22 and name H2" )( resid 22 and name H8 ) 3.70 0.57 0.58 !9
!assign ( resid 22 and name H2' )( resid 22 and name H1' ) 2.16 0.25 0.25 !325
!assign ( resid 22 and name H1' )( resid 22 and name H4' ) 2.46 0.31 0.31 !352
assign ( resid 16 and name H2' )( resid 17 and name H5# ) 2.90 0.57 0.58 !478
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set message=on echo=on end

Table S4. Restraints for the b-R(61,2) adduct

R-styrene

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set message=off echo=off end
assign ( resid 2 and name H8 )( resid 2 and name H1' ) 3.26 0.65 0.66
assign ( resid 3 and name H8 )( resid 3 and name H1' ) 3.38 0.51 0.51
assign ( resid 4 and name H8 )( resid 4 and name H1' ) 3.59 0.70 0.71
assign ( resid 5 and name H6 )( resid 5 and name H1' ) 4.00 0.47 0.46
assign ( resid 6 and name H8 )( resid 6 and name H1' ) 3.80 0.56 0.56
assign ( resid 7 and name H8 )( resid 7 and name H1' ) 3.33 0.61 0.62
assign ( resid 8 and name H8 )( resid 8 and name H1' ) 3.41 0.63 0.62
assign ( resid 10 and name H8 )( resid 10 and name H1' ) 3.41 0.51 0.50
assign ( resid 12 and name H6 )( resid 12 and name H1' ) 2.96 0.69 0.70
assign ( resid 13 and name H6 )( resid 13 and name H1' ) 2.79 0.89 0.89
assign ( resid 14 and name H6 )( resid 14 and name H1' ) 3.02 0.94 0.94
assign ( resid 16 and name H6 )( resid 16 and name H1' ) 3.57 0.63 0.62
assign ( resid 17 and name H6 )( resid 17 and name H1' ) 3.25 0.71 0.71
assign ( resid 18 and name H8 )( resid 18 and name H1' ) 3.29 0.85 0.85
assign ( resid 22 and name H8 )( resid 22 and name H1' ) 3.82 0.38 0.38
assign ( resid 2 and name H8 )( resid 1 and name H1' ) 3.87 1.08 1.08
assign ( resid 3 and name H8 )( resid 2 and name H1' ) 2.91 0.35 0.34
assign ( resid 4 and name H8 )( resid 3 and name H1' ) 3.11 0.36 0.36
assign ( resid 5 and name H6 )( resid 4 and name H1' ) 3.43 0.83 0.83
assign ( resid 6 and name H8 )( resid 5 and name H1' ) 3.25 0.46 0.46
assign ( resid 7 and name H8 )( resid 6 and name H1' ) 3.10 0.46 0.46
assign ( resid 9 and name H8 )( resid 8 and name H1' ) 3.07 0.50 0.50
assign ( resid 14 and name H6 )( resid 13 and name H1' ) 3.00 0.79 0.79
assign ( resid 15 and name H6 )( resid 14 and name H1' ) 3.49 0.94 0.94
assign ( resid 16 and name H6 )( resid 15 and name H1' ) 3.33 0.71 0.71
assign ( resid 17 and name H6 )( resid 16 and name H1' ) 3.76 1.18 1.18
assign ( resid 18 and name H8 )( resid 17 and name H1' ) 3.06 0.65 0.65
assign ( resid 22 and name H8 )( resid 21 and name H1' ) 3.73 0.90 0.90
assign ( resid 2 and name H8 )( resid 1 and name H2' ) 3.00 0.69 0.70
assign ( resid 5 and name H6 )( resid 4 and name H2' ) 3.54 0.48 0.47
assign ( resid 6 and name H8 )( resid 5 and name H2' ) 3.73 0.40 0.40
assign ( resid 18 and name H8 )( resid 17 and name H2' ) 3.82 0.73 0.73
assign ( resid 22 and name H8 )( resid 21 and name H2' ) 3.42 0.38 0.38
assign ( resid 5 and name H6 )( resid 4 and name H2'' ) 2.75 0.69 0.69
assign ( resid 6 and name H8 )( resid 5 and name H2'' ) 3.34 1.09 1.09
assign ( resid 8 and name H8 )( resid 7 and name H2'' ) 3.35 1.05 1.05
assign ( resid 11 and name H8 )( resid 10 and name H2'' ) 2.87 0.55 0.54
assign ( resid 17 and name H6 )( resid 16 and name H2'' ) 2.67 0.53 0.53
assign ( resid 19 and name H6 )( resid 18 and name H2'' ) 2.69 0.57 0.57
assign ( resid 1 and name H2' )( resid 1 and name H6 ) 2.40 0.49 0.50
assign ( resid 5 and name H2' )( resid 5 and name H6 ) 2.47 0.57 0.58
assign ( resid 21 and name H2' )( resid 21 and name H6 ) 2.26 0.39 0.39
assign ( resid 22 and name H2' )( resid 22 and name H8 ) 2.34 0.23 0.23

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assign ( resid 5 and name H2" )( resid 5 and name H6 ) 2.83 0.58 0.58
assign ( resid 17 and name H2" )( resid 17 and name H6 ) 2.85 0.55 0.55
assign ( resid 18 and name H2" )( resid 18 and name H8 ) 2.73 0.93 0.94
assign ( resid 1 and name H3' )( resid 1 and name H6 ) 2.75 1.29 1.29
assign ( resid 2 and name H3' )( resid 2 and name H8 ) 3.35 1.05 1.05
assign ( resid 3 and name H3' )( resid 3 and name H8 ) 3.52 0.83 0.83
assign ( resid 5 and name H3' )( resid 5 and name H6 ) 3.66 0.66 0.66
assign ( resid 6 and name H3' )( resid 6 and name H8 ) 3.44 0.94 0.94
assign ( resid 8 and name H3' )( resid 8 and name H8 ) 3.77 0.60 0.60
assign ( resid 11 and name H3' )( resid 11 and name H8 ) 3.58 0.87 0.87
assign ( resid 13 and name H3' )( resid 13 and name H6 ) 3.04 0.98 0.97
assign ( resid 22 and name H3' )( resid 22 and name H8 ) 3.25 1.12 1.12
assign ( resid 8 and name H8 )( resid 7 and name H3' ) 4.39 0.81 0.82
assign ( resid 11 and name H8 )( resid 10 and name H3' ) 4.77 0.82 0.81
assign ( resid 13 and name H6 )( resid 12 and name H3' ) 3.30 1.50 1.50
assign ( resid 1 and name H5' )( resid 1 and name H6 ) 3.82 0.61 0.61
assign ( resid 11 and name H5' )( resid 11 and name H8 ) 3.29 0.42 0.42
assign ( resid 12 and name H5' )( resid 12 and name H6 ) 3.17 0.65 0.65
assign ( resid 13 and name H5' )( resid 13 and name H6 ) 3.21 0.60 0.60
assign ( resid 22 and name H5' )( resid 22 and name H8 ) 3.62 0.58 0.58
assign ( resid 13 and name H5# )( resid 12 and name H6 ) 3.64 0.56 0.56
assign ( resid 16 and name H5# )( resid 15 and name H6 ) 3.47 0.35 0.35
assign ( ( resid 6 and name HS1 ) or ( resid 6 and name HS5 )
      ( resid 16 and name H5# ) 4.19 0.42 0.42
assign ( resid 17 and name H5# )( resid 17 and name H6 ) 2.43 0.82 0.81
assign ( resid 19 and name H5# )( resid 18 and name H8 ) 3.48 0.43 0.43
assign ( resid 19 and name H5# )( resid 19 and name H6 ) 2.54 0.68 0.67
assign ( resid 12 and name H5 )( resid 13 and name H5# ) 3.89 0.77 0.77
assign ( resid 15 and name H5 )( resid 14 and name H5# ) 4.75 0.55 0.55
assign ( resid 16 and name H5# )( resid 15 and name H5 ) 4.25 0.43 0.43
assign ( resid 20 and name H5 )( resid 19 and name H5# ) 5.13 0.68 0.68
assign ( resid 13 and name H5# )( resid 12 and name H1' ) 4.62 0.98 0.97
assign ( resid 14 and name H5# )( resid 13 and name H1' ) 5.07 1.07 1.07
assign ( resid 16 and name H5# )( resid 15 and name H1' ) 5.29 1.31 1.31
assign ( resid 17 and name H5# )( resid 16 and name H1' ) 5.05 1.07 1.08
assign ( resid 19 and name H5# )( resid 18 and name H1' ) 5.34 1.33 1.33
assign ( resid 17 and name H5# )( resid 16 and name H2' ) 3.54 0.67 0.67
assign ( resid 19 and name H5# )( resid 18 and name H2' ) 3.50 0.58 0.58
assign ( resid 17 and name H5# )( resid 16 and name H2" ) 3.71 0.94 0.94
assign ( resid 19 and name H5# )( resid 18 and name H2" ) 3.71 0.87 0.87
assign ( resid 13 and name H5# )( resid 12 and name H3' ) 3.03 1.00 1.00
assign ( resid 1 and name H5 )( resid 1 and name H2' ) 3.27 1.02 1.02
assign ( resid 21 and name H5 )( resid 20 and name H2' ) 3.96 0.81 0.81
assign ( resid 21 and name H2' )( resid 21 and name H5 ) 3.82 0.73 0.73
assign ( resid 15 and name H5 )( resid 14 and name H2" ) 3.26 0.56 0.56
assign ( resid 20 and name H5 )( resid 19 and name H2" ) 3.04 0.40 0.40

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assign ( resid 5 and name H5 )( resid 4 and name H8 ) 3.71 0.37 0.37
assign ( resid 20 and name H5 )( resid 19 and name H6 ) 4.10 0.41 0.41
assign ( resid 10 and name H2 )( resid 11 and name H1' ) 3.85 0.73 0.73
assign ( resid 15 and name H5 )( resid 14 and name H2' ) 3.49 0.38 0.38
assign ( resid 1 and name H2' )( resid 1 and name H1' ) 2.86 0.62 0.62
assign ( resid 3 and name H2' )( resid 3 and name H1' ) 3.08 0.39 0.38
assign ( resid 5 and name H2' )( resid 5 and name H1' ) 2.98 0.44 0.44
assign ( resid 8 and name H2' )( resid 8 and name H1' ) 3.16 0.38 0.38
assign ( resid 12 and name H2' )( resid 12 and name H1' ) 2.46 0.52 0.53
assign ( resid 13 and name H2' )( resid 13 and name H1' ) 2.89 0.55 0.55
assign ( resid 17 and name H2' )( resid 17 and name H1' ) 3.35 0.46 0.46
assign ( resid 21 and name H2' )( resid 21 and name H1' ) 2.89 0.51 0.51
assign ( resid 1 and name H2'' )( resid 1 and name H1' ) 2.26 0.25 0.25
assign ( resid 3 and name H2'' )( resid 3 and name H1' ) 2.25 0.22 0.22
assign ( resid 4 and name H2'' )( resid 4 and name H1' ) 2.26 0.23 0.23
assign ( resid 5 and name H2'' )( resid 5 and name H1' ) 2.39 0.24 0.24
assign ( resid 8 and name H2'' )( resid 8 and name H1' ) 2.23 0.22 0.22
assign ( resid 9 and name H2'' )( resid 9 and name H1' ) 2.68 0.36 0.37
assign ( resid 17 and name H2'' )( resid 17 and name H1' ) 2.27 0.23 0.23
assign ( resid 18 and name H2'' )( resid 18 and name H1' ) 2.25 0.28 0.27
assign ( resid 21 and name H2'' )( resid 21 and name H1' ) 2.29 0.23 0.23
assign ( resid 22 and name H2'' )( resid 22 and name H1' ) 2.38 0.24 0.24
assign ( resid 1 and name H3' )( resid 1 and name H1' ) 4.39 0.83 0.83
assign ( resid 2 and name H3' )( resid 2 and name H1' ) 3.40 0.63 0.63
assign ( resid 3 and name H3' )( resid 3 and name H1' ) 3.75 0.60 0.59
assign ( resid 4 and name H3' )( resid 4 and name H1' ) 3.87 0.69 0.69
assign ( resid 5 and name H3' )( resid 5 and name H1' ) 4.04 0.60 0.60
assign ( resid 6 and name H3' )( resid 6 and name H1' ) 3.71 0.77 0.78
assign ( resid 7 and name H3' )( resid 7 and name H1' ) 3.60 0.82 0.83
assign ( resid 8 and name H3' )( resid 8 and name H1' ) 3.29 0.69 0.69
assign ( resid 9 and name H3' )( resid 9 and name H1' ) 3.95 0.73 0.73
assign ( resid 10 and name H3' )( resid 10 and name H1' ) 3.60 0.75 0.75
assign ( resid 11 and name H3' )( resid 11 and name H1' ) 3.89 0.46 0.46
assign ( resid 12 and name H3' )( resid 12 and name H1' ) 3.79 0.73 0.72
assign ( resid 13 and name H3' )( resid 13 and name H1' ) 3.42 0.63 0.63
assign ( resid 17 and name H3' )( resid 17 and name H1' ) 3.75 0.69 0.68
assign ( resid 18 and name H3' )( resid 18 and name H1' ) 3.42 0.96 0.96
assign ( resid 22 and name H3' )( resid 22 and name H1' ) 4.04 0.54 0.54
assign ( resid 1 and name H1' )( resid 1 and name H4' ) 2.71 0.99 0.99
assign ( resid 2 and name H1' )( resid 2 and name H4' ) 3.12 0.62 0.62
assign ( resid 3 and name H4' )( resid 3 and name H1' ) 3.36 0.37 0.36
assign ( resid 4 and name H4' )( resid 4 and name H1' ) 3.11 0.58 0.58
assign ( resid 6 and name H4' )( resid 6 and name H1' ) 3.33 0.38 0.39
assign ( resid 8 and name H4' )( resid 8 and name H1' ) 2.88 0.86 0.86
assign ( resid 12 and name H1' )( resid 12 and name H4' ) 2.70 1.00 1.00
assign ( resid 13 and name H4' )( resid 13 and name H1' ) 2.81 0.91 0.91

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assign ( resid 9 and name H5' )( resid 8 and name H1' ) 3.13 0.25 0.25
assign ( resid 1 and name H3' )( resid 1 and name H2' ) 2.28 0.28 0.28
assign ( resid 22 and name H3' )( resid 22 and name H2' ) 2.60 0.26 0.26
assign ( resid 20 and name H2'' )( resid 20 and name H2' ) 2.08 0.24 0.24
assign ( resid 21 and name H2'' )( resid 21 and name H2' ) 2.15 0.35 0.35
assign ( resid 11 and name H4' )( resid 11 and name H3' ) 2.99 0.42 0.42
assign ( resid 22 and name H4' )( resid 22 and name H3' ) 2.72 0.27 0.27
assign ( resid 1 and name H5' )( resid 1 and name H3' ) 2.58 1.22 1.22
assign ( resid 2 and name H5' )( resid 2 and name H3' ) 2.87 0.89 0.89
assign ( resid 12 and name H5' )( resid 12 and name H3' ) 2.48 1.36 1.36
assign ( resid 1 and name H5' )( resid 1 and name H4' ) 2.23 0.41 0.40
assign ( resid 12 and name H5' )( resid 12 and name H4' ) 1.96 0.50 0.50
assign ( resid 6 and name HB' )( resid 6 and name HB'' ) 1.80 0.21 0.21
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS5 ))
      ( resid 6 and name HB'' ) 3.50 0.78 0.79
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS2 )
      or ( resid 6 and name HS3 ) or ( resid 6 and name HS4 ))
      ( resid 6 and name HB'' ) 4.72 0.78 0.79
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS5 ))
      ( resid 6 and name HB' ) 3.50 0.78 0.79
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS2 )
      or ( resid 6 and name HS3 ) or ( resid 6 and name HS4 ))
      ( resid 6 and name HB' ) 5.00 0.78 0.79
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS5 ))
      ( resid 6 and name HA ) 3.00 0.78 0.79
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS2 )
      or ( resid 6 and name HS3 ) or ( resid 6 and name HS4 ))
      ( resid 6 and name HA ) 4.52 0.78 0.79
assign ( resid 6 and name HB' )( resid 5 and name H5 ) 4.50 0.50 0.50
assign ( resid 6 and name HB'' )( resid 6 and name H8 ) 5.50 0.50 0.50
assign ( resid 6 and name HB' )( resid 6 and name H8 ) 4.90 0.70 0.70
assign ( resid 6 and name HA )( resid 6 and name H8 ) 5.50 0.50 0.50
assign ( resid 6 and name HB' )( resid 5 and name H6 ) 5.50 0.70 0.70
assign ( resid 6 and name HA )( resid 5 and name H5 ) 6.00 1.00 1.00
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS5 ))
      ( resid 6 and name H8 ) 5.50 0.78 0.79
assign (( resid 6 and name HS2 ) or ( resid 6 and name HS4 ))
      ( resid 6 and name H8 ) 5.50 0.78 0.79
assign ( resid 6 and name HB'' )( resid 5 and name H5 ) 3.67 0.43 0.43
assign ( resid 6 and name HA )( resid 6 and name HB' ) 2.50 0.35 0.35
assign ( resid 5 and name H5 )( resid 6 and name HS# ) 5.50 0.50 0.50
!assign ( resid 6 and name H8 )( resid 5 and name H6 ) 4.30 0.50 0.50
!assign ( resid 4 and name H8 )( resid 5 and name H6 ) 3.80 0.50 0.50
assign (( resid 6 and name HS1 ) or ( resid 6 and name HS2 ))
      ( resid 5 and name H6 ) 4.00 0.78 0.79

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!Water NOE peaks estimated

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assign ( resid 6 and name HB" )( resid 5 and name H4# ) 3.67 1.00 1.00
assign ( resid 6 and name H6 )( resid 6 and name HB" ) 2.50 1.00 1.00
assign ( resid 6 and name H6 )( resid 6 and name HB' ) 2.80 1.00 1.00
assign ( resid 6 and name HB" )( resid 17 and name H3 ) 4.00 1.00 1.00
assign ( resid 18 and name H1 )( resid 6 and name HB" ) 4.50 1.00 1.00
assign ( resid 17 and name H3 )( resid 6 and name HB' ) 4.50 1.00 1.00

```

!Water theoretical restrains

```

assign ( resid 11 and name H1 )( resid 13 and name H3 ) 3.38 0.20 0.20
assign ( resid 13 and name H3 )( resid 14 and name H3 ) 3.49 0.10 0.10
assign ( resid 14 and name H3 )( resid 8 and name H1 ) 3.73 0.10 0.10
assign ( resid 8 and name H1 )( resid 16 and name H3 ) 3.38 0.10 0.10
assign ( resid 16 and name H3 )( resid 17 and name H3 ) 3.49 0.10 0.10
assign ( resid 17 and name H3 )( resid 18 and name H1 ) 4.13 0.10 0.10
assign ( resid 18 and name H1 )( resid 19 and name H3 ) 3.49 0.10 0.10
assign ( resid 19 and name H3 )( resid 3 and name H1 ) 3.73 0.10 0.10
assign ( resid 3 and name H1 )( resid 2 and name H1 ) 3.41 0.10 0.10
assign ( resid 2 and name H1 )( resid 22 and name H1 ) 3.71 0.20 0.20

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!More Water theoretical restrains

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assign ( resid 21 and name H41 )( resid 3 and name H1 ) 3.88 0.10 0.10
assign ( resid 20 and name H41 )( resid 2 and name H1 ) 4.43 0.10 0.10
assign ( resid 20 and name H41 )( resid 19 and name H3 ) 3.60 0.10 0.10
assign ( resid 18 and name H1 )( resid 6 and name H2 ) 3.96 0.10 0.10
assign ( resid 18 and name H1 )( resid 4 and name H2 ) 3.81 0.10 0.10
assign ( resid 17 and name H3 )( resid 7 and name H2 ) 3.92 0.10 0.10
assign ( resid 7 and name H2 )( resid 8 and name H1 ) 4.32 0.10 0.10
assign ( resid 8 and name H1 )( resid 9 and name H2 ) 3.92 0.10 0.10
assign ( resid 9 and name H61 )( resid 13 and name H3 ) 3.92 0.10 0.10
assign ( resid 14 and name H3 )( resid 15 and name H41 ) 3.60 0.10 0.10
assign ( resid 16 and name H3 )( resid 15 and name H41 ) 4.49 0.10 0.10

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set message=on echo=on end

set message=off echo=off end

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assign ( resid 1 and name H6 )( resid 1 and name H1' ) 2.64 1.07 1.07
assign ( resid 9 and name H8 )( resid 9 and name H1' ) 3.53 0.35 0.35
assign ( resid 19 and name H6 )( resid 19 and name H1' ) 3.72 0.52 0.52
assign ( resid 20 and name H6 )( resid 20 and name H1' ) 3.62 0.44 0.43
assign ( resid 21 and name H6 )( resid 21 and name H1' ) 3.58 0.36 0.36
assign ( resid 8 and name H8 )( resid 7 and name H1' ) 3.19 0.48 0.48
assign ( resid 10 and name H8 )( resid 9 and name H1' ) 3.15 0.38 0.38
assign ( resid 13 and name H6 )( resid 12 and name H1' ) 3.05 0.74 0.74
assign ( resid 21 and name H6 )( resid 20 and name H1' ) 4.02 1.40 1.40
assign ( resid 2 and name H8 )( resid 1 and name H2" ) 2.90 0.62 0.62
assign ( resid 16 and name H6 )( resid 15 and name H2" ) 2.79 0.68 0.67
assign ( resid 21 and name H6 )( resid 20 and name H2" ) 3.08 0.97 0.96

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assign ( resid 6 and name H2' )( resid 6 and name H8 ) 2.25 0.24 0.23
assign ( resid 19 and name H2' )( resid 19 and name H6 ) 2.40 0.52 0.52
assign ( resid 2 and name H2'' )( resid 2 and name H8 ) 2.75 0.98 0.98
assign ( resid 6 and name H2'' )( resid 6 and name H8 ) 3.13 0.59 0.59
assign ( resid 16 and name H2'' )( resid 16 and name H6 ) 2.51 0.92 0.92
assign ( resid 15 and name H3' )( resid 15 and name H6 ) 3.21 0.84 0.84
assign ( resid 16 and name H3' )( resid 16 and name H6 ) 3.13 0.85 0.85
assign ( resid 20 and name H3' )( resid 20 and name H6 ) 3.25 0.71 0.71
assign ( resid 3 and name H8 )( resid 2 and name H3' ) 5.12 0.88 0.88
assign ( resid 5 and name H6 )( resid 4 and name H3' ) 4.00 0.83 0.83
assign ( resid 6 and name H8 )( resid 5 and name H3' ) 5.87 1.05 1.05
assign ( resid 1 and name H6 )( resid 1 and name H4' ) 4.55 1.01 1.02
assign ( resid 2 and name H8 )( resid 2 and name H4' ) 3.65 1.22 1.22
assign ( resid 3 and name H4' )( resid 3 and name H8 ) 3.84 1.03 1.04
assign ( resid 6 and name H4' )( resid 6 and name H8 ) 3.40 1.50 1.50
assign ( resid 7 and name H4' )( resid 7 and name H8 ) 3.95 0.72 0.72
assign ( resid 8 and name H4' )( resid 8 and name H8 ) 4.00 0.94 0.93
assign ( resid 11 and name H4' )( resid 11 and name H8 ) 5.36 0.77 0.77
assign ( resid 12 and name H6 )( resid 12 and name H4' ) 3.87 0.85 0.84
assign ( resid 13 and name H4' )( resid 13 and name H6 ) 4.42 0.89 0.89
assign ( resid 14 and name H4' )( resid 14 and name H6 ) 4.39 0.73 0.73
assign ( resid 16 and name H4' )( resid 16 and name H6 ) 4.44 0.90 0.89
assign ( resid 18 and name H4' )( resid 18 and name H8 ) 4.48 0.64 0.64
assign ( resid 19 and name H4' )( resid 19 and name H6 ) 4.42 0.96 0.96
assign ( resid 22 and name H4' )( resid 22 and name H8 ) 4.16 1.45 1.45
assign ( resid 2 and name H8 )( resid 1 and name H4' ) 5.01 1.04 1.04
assign ( resid 17 and name H4' )( resid 18 and name H8 ) 4.73 1.24 1.24
assign ( resid 4 and name H5' )( resid 4 and name H8 ) 3.66 0.56 0.56
assign ( resid 6 and name H5' )( resid 6 and name H8 ) 3.50 0.85 0.85
assign ( resid 8 and name H5' )( resid 8 and name H8 ) 3.49 0.76 0.75
assign ( resid 9 and name H5' )( resid 9 and name H8 ) 3.67 0.67 0.67
assign ( resid 10 and name H5' )( resid 10 and name H8 ) 3.59 0.79 0.79
assign ( resid 14 and name H5' )( resid 14 and name H6 ) 3.63 0.70 0.70
assign ( resid 18 and name H5' )( resid 18 and name H8 ) 3.96 0.85 0.86
assign ( resid 19 and name H5' )( resid 19 and name H6 ) 2.72 0.67 0.67
assign ( resid 13 and name H5# )( resid 13 and name H6 ) 2.31 0.90 0.90
assign ( resid 14 and name H5# )( resid 13 and name H6 ) 3.12 0.59 0.59
assign ( resid 14 and name H5# )( resid 14 and name H6 ) 2.38 0.76 0.77
assign ( resid 17 and name H5# )( resid 16 and name H6 ) 3.36 0.45 0.45
assign ( resid 16 and name H5# )( resid 15 and name H2' ) 3.27 0.33 0.33
assign ( resid 14 and name H5# )( resid 13 and name H2'' ) 3.58 0.75 0.75
assign ( resid 16 and name H5# )( resid 15 and name H2'' ) 4.03 1.26 1.25
assign ( resid 16 and name H5# )( resid 15 and name H3' ) 4.52 0.65 0.65
!assign ( resid 13 and name H5# )( resid 13 and name H5' ) 4.50 0.50 0.50
assign ( resid 19 and name H2' )( resid 19 and name H5# ) 4.29 1.17 1.17
assign ( resid 13 and name H3' )( resid 14 and name H5# ) 4.21 0.80 0.80

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assign ( resid 16 and name H3' )( resid 16 and name H5# ) 5.44 1.12 1.12
assign ( resid 16 and name H3' )( resid 17 and name H5# ) 4.52 0.50 0.50
assign ( resid 18 and name H3' )( resid 19 and name H5# ) 4.65 0.65 0.65
assign ( resid 15 and name H1' )( resid 9 and name H2 ) 3.69 0.37 0.37
assign ( resid 18 and name H1' )( resid 6 and name H2 ) 4.62 0.46 0.46
assign ( resid 20 and name H1' )( resid 4 and name H2 ) 4.37 0.44 0.44
assign ( resid 7 and name H2 )( resid 17 and name H1' ) 4.63 0.46 0.46
assign ( resid 10 and name H2 )( resid 14 and name H1' ) 4.14 0.41 0.41
assign ( resid 5 and name H5 )( resid 4 and name H2' ) 4.51 1.32 1.33
assign ( resid 5 and name H2' )( resid 5 and name H5 ) 4.02 0.73 0.72
assign ( resid 15 and name H2' )( resid 15 and name H5 ) 3.28 1.04 1.04
assign ( resid 5 and name H5 )( resid 4 and name H2" ) 3.47 0.68 0.68
assign ( resid 21 and name H5 )( resid 20 and name H2" ) 3.74 0.81 0.81
!assign ( resid 5 and name H3' )( resid 6 and name HA ) 3.40 0.60 0.60
assign ( resid 15 and name H5 )( resid 14 and name H6 ) 4.04 0.51 0.50
assign ( resid 4 and name H2 )( resid 4 and name H1' ) 5.77 1.26 1.26
assign ( resid 6 and name H2 )( resid 6 and name H1' ) 4.89 0.49 0.49
assign ( resid 6 and name H2' )( resid 6 and name H1' ) 2.99 0.36 0.36
assign ( resid 15 and name H2' )( resid 15 and name H1' ) 3.51 0.79 0.79
assign ( resid 19 and name H2' )( resid 19 and name H1' ) 2.63 0.54 0.55
assign ( resid 20 and name H2' )( resid 20 and name H1' ) 2.73 0.52 0.52
assign ( resid 2 and name H2" )( resid 2 and name H1' ) 2.12 0.22 0.21
assign ( resid 6 and name H2" )( resid 6 and name H1' ) 2.27 0.23 0.23
assign ( resid 11 and name H2" )( resid 11 and name H1' ) 2.29 0.23 0.23
assign ( resid 20 and name H2" )( resid 20 and name H1' ) 2.30 0.23 0.23
assign ( resid 15 and name H3' )( resid 15 and name H1' ) 3.19 0.73 0.73
assign ( resid 19 and name H3' )( resid 19 and name H1' ) 4.04 0.60 0.59
assign ( resid 5 and name H4' )( resid 5 and name H1' ) 3.60 0.36 0.36
assign ( resid 4 and name H5' )( resid 3 and name H1' ) 3.00 0.40 0.40
assign ( resid 21 and name H5' )( resid 20 and name H1' ) 3.10 0.40 0.40
assign ( resid 5 and name H3' )( resid 5 and name H2' ) 2.71 0.27 0.27
assign ( resid 11 and name H3' )( resid 11 and name H2' ) 2.51 0.25 0.25
assign ( resid 15 and name H3' )( resid 15 and name H2' ) 2.27 0.23 0.23
assign ( resid 21 and name H3' )( resid 21 and name H2' ) 3.10 0.76 0.76
assign ( resid 11 and name H3' )( resid 11 and name H2" ) 3.02 0.31 0.31
assign ( resid 12 and name H3' )( resid 12 and name H2" ) 3.59 0.94 0.95
assign ( resid 15 and name H3' )( resid 15 and name H2" ) 3.87 1.15 1.15
assign ( resid 20 and name H3' )( resid 20 and name H2" ) 3.25 0.71 0.71
assign ( resid 1 and name H2' )( resid 1 and name H4' ) 3.92 0.99 0.99
assign ( resid 5 and name H4' )( resid 5 and name H2' ) 4.17 0.79 0.79
assign ( resid 21 and name H4' )( resid 21 and name H2' ) 4.11 0.95 0.95
assign ( resid 1 and name H5' )( resid 1 and name H2' ) 3.78 0.84 0.83
assign ( resid 18 and name H4' )( resid 18 and name H3' ) 2.67 0.30 0.31
assign ( resid 5 and name H1' )( resid 6 and name H5' ) 3.60 0.35 0.36

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set message=on echo=on end

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set message=off echo=off end
assign ( resid 15 and name H6 )( resid 15 and name H1' ) 3.29 0.54 0.54
assign ( resid 20 and name H6 )( resid 19 and name H1' ) 3.31 0.77 0.77
assign ( resid 7 and name H8 )( resid 6 and name H2' ) 3.31 0.50 0.50
assign ( resid 14 and name H6 )( resid 13 and name H2'' ) 2.70 0.62 0.61
assign ( resid 22 and name H8 )( resid 21 and name H2'' ) 3.17 0.88 0.88
assign ( resid 2 and name H2' )( resid 2 and name H8 ) 2.15 0.25 0.25
assign ( resid 7 and name H2' )( resid 7 and name H8 ) 2.13 0.21 0.21
assign ( resid 8 and name H2' )( resid 8 and name H8 ) 2.23 0.22 0.22
assign ( resid 12 and name H2' )( resid 12 and name H6 ) 2.42 0.49 0.48
assign ( resid 15 and name H2' )( resid 15 and name H6 ) 2.38 0.46 0.46
assign ( resid 12 and name H2'' )( resid 12 and name H6 ) 3.32 0.77 0.77
assign ( resid 20 and name H2'' )( resid 20 and name H6 ) 3.00 0.82 0.81
assign ( resid 21 and name H2'' )( resid 21 and name H6 ) 2.54 0.90 0.90
assign ( resid 22 and name H2'' )( resid 22 and name H8 ) 2.84 0.86 0.87
assign ( resid 12 and name H3' )( resid 12 and name H6 ) 2.82 1.19 1.19
assign ( resid 2 and name H8 )( resid 1 and name H3' ) 3.11 1.77 1.77
assign ( resid 15 and name H6 )( resid 14 and name H3' ) 3.92 0.91 0.91
assign ( resid 20 and name H6 )( resid 19 and name H3' ) 5.05 0.79 0.79
assign ( resid 4 and name H4' )( resid 4 and name H8 ) 5.01 0.80 0.80
assign ( resid 16 and name H5# )( resid 16 and name H6 ) 2.66 0.58 0.58
assign ( resid 13 and name H5# )( resid 12 and name H2' ) 3.00 0.59 0.59
assign ( resid 13 and name H5# )( resid 12 and name H2'' ) 4.15 1.40 1.40
assign ( resid 20 and name H5 )( resid 19 and name H2' ) 3.81 0.61 0.61
assign ( resid 20 and name H2' )( resid 20 and name H5 ) 3.36 1.01 1.00
assign ( resid 20 and name H5 )( resid 19 and name H3' ) 4.27 1.26 1.26
assign ( resid 11 and name H3' )( resid 11 and name H5'' ) 2.42 0.31 0.31
assign ( resid 7 and name H2 )( resid 8 and name H1' ) 2.87 1.69 1.69
assign ( resid 2 and name H2' )( resid 2 and name H1' ) 2.96 0.54 0.54
assign ( resid 11 and name H2' )( resid 11 and name H1' ) 3.16 0.49 0.48
assign ( resid 14 and name H2' )( resid 14 and name H1' ) 3.12 0.58 0.58
assign ( resid 16 and name H2' )( resid 16 and name H1' ) 2.44 0.51 0.51
assign ( resid 12 and name H2'' )( resid 12 and name H1' ) 2.05 0.23 0.23
assign ( resid 15 and name H2'' )( resid 15 and name H1' ) 2.00 0.26 0.25
assign ( resid 16 and name H2'' )( resid 16 and name H1' ) 2.31 0.23 0.23
assign ( resid 9 and name H4' )( resid 9 and name H1' ) 3.06 0.62 0.62
assign ( resid 18 and name H4' )( resid 18 and name H1' ) 2.99 0.68 0.68
assign ( resid 21 and name H4' )( resid 21 and name H1' ) 2.77 0.90 0.90
assign ( resid 6 and name H5' )( resid 5 and name H1' ) 3.23 0.35 0.35
assign ( resid 10 and name H5' )( resid 9 and name H1' ) 2.37 0.50 0.50
assign ( resid 22 and name H5' )( resid 21 and name H1' ) 3.08 0.40 0.40
assign ( resid 8 and name H3' )( resid 8 and name H2' ) 2.60 0.32 0.32
assign ( resid 5 and name H3' )( resid 5 and name H2'' ) 2.83 0.33 0.32
assign ( resid 7 and name H3' )( resid 7 and name H2'' ) 2.43 0.36 0.37
assign ( resid 18 and name H3' )( resid 18 and name H2'' ) 3.33 0.82 0.82

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assign ( resid 21 and name H3' )( resid 21 and name H2" ) 3.22 0.51 0.51
assign ( resid 22 and name H3' )( resid 22 and name H2" ) 3.07 0.42 0.42
assign ( resid 6 and name H4' )( resid 6 and name H3' ) 2.45 0.35 0.35
assign ( resid 7 and name H4' )( resid 7 and name H3' ) 2.38 0.29 0.30
assign ( resid 12 and name H3' )( resid 12 and name H4' ) 2.50 0.49 0.49
assign ( resid 22 and name H5' )( resid 22 and name H3' ) 3.80 0.20 0.20
assign ( resid 2 and name H5' )( resid 2 and name H4' ) 1.98 0.47 0.47
assign ( resid 1 and name H3' )( resid 1 and name H4' ) 2.60 0.20 0.20

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set message=on echo=on end

set message=off echo=off end

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assign ( resid 15 and name H6 )( resid 14 and name H2' ) 3.06 0.53 0.53
assign ( resid 7 and name H8 )( resid 6 and name H2" ) 2.62 0.31 0.31
assign ( resid 20 and name H2" )( resid 20 and name H6 ) 2.25 0.31 0.30
assign ( resid 7 and name H2" )( resid 7 and name H8 ) 3.08 0.59 0.60
assign ( resid 9 and name H2" )( resid 9 and name H8 ) 3.00 1.20 1.21
assign ( resid 11 and name H2" )( resid 11 and name H8 ) 2.94 0.73 0.73
assign ( resid 14 and name H2" )( resid 14 and name H6 ) 3.40 0.68 0.68
assign ( resid 7 and name H2' )( resid 7 and name H1' ) 3.30 0.65 0.65
assign ( resid 19 and name H4' )( resid 19 and name H1' ) 2.58 1.11 1.12
assign ( resid 20 and name H4' )( resid 20 and name H1' ) 2.66 1.04 1.04
assign ( resid 22 and name H4' )( resid 22 and name H1' ) 2.96 0.73 0.73
assign ( resid 7 and name H3' )( resid 7 and name H2' ) 2.43 0.36 0.37
assign ( resid 18 and name H3' )( resid 18 and name H2' ) 2.05 0.48 0.48
assign ( resid 8 and name H3' )( resid 8 and name H2" ) 2.34 0.40 0.40
assign ( resid 16 and name H2" )( resid 16 and name H2' ) 2.07 0.29 0.29
assign ( resid 3 and name H4' )( resid 3 and name H3' ) 2.06 0.80 0.80

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set message=on echo=on end

set message=off echo=off end

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assign ( resid 11 and name H8 )( resid 11 and name H1' ) 3.47 0.63 0.63
assign ( resid 11 and name H8 )( resid 10 and name H1' ) 3.61 0.84 0.83
assign ( resid 19 and name H6 )( resid 18 and name H1' ) 3.03 0.62 0.61
assign ( resid 3 and name H8 )( resid 2 and name H2' ) 2.95 0.79 0.78
assign ( resid 4 and name H8 )( resid 3 and name H2' ) 2.72 0.99 0.99
assign ( resid 8 and name H8 )( resid 7 and name H2' ) 2.34 1.31 1.31
assign ( resid 9 and name H8 )( resid 8 and name H2' ) 2.96 0.69 0.69
assign ( resid 10 and name H8 )( resid 9 and name H2' ) 2.96 0.74 0.75
assign ( resid 11 and name H8 )( resid 10 and name H2' ) 3.24 0.51 0.51
assign ( resid 14 and name H6 )( resid 13 and name H2' ) 2.56 1.06 1.06
assign ( resid 16 and name H6 )( resid 15 and name H2' ) 2.73 0.86 0.86
assign ( resid 17 and name H6 )( resid 16 and name H2' ) 2.54 1.02 1.02
assign ( resid 19 and name H6 )( resid 18 and name H2' ) 3.31 0.67 0.67
assign ( resid 21 and name H6 )( resid 20 and name H2' ) 2.60 0.96 0.96

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assign ( resid 3 and name H8 )( resid 2 and name H2" ) 2.99 0.68 0.67
assign ( resid 4 and name H8 )( resid 3 and name H2" ) 3.26 0.96 0.96
assign ( resid 10 and name H8 )( resid 9 and name H2" ) 3.02 0.77 0.77
assign ( resid 13 and name H6 )( resid 12 and name H2" ) 2.79 0.67 0.67
assign ( resid 15 and name H6 )( resid 14 and name H2" ) 2.87 0.76 0.75
assign ( resid 18 and name H8 )( resid 17 and name H2" ) 2.53 0.27 0.27
assign ( resid 20 and name H6 )( resid 19 and name H2" ) 2.75 0.62 0.62
assign ( resid 3 and name H2' )( resid 3 and name H8 ) 2.32 0.26 0.26
assign ( resid 4 and name H2' )( resid 4 and name H8 ) 2.35 0.25 0.25
assign ( resid 9 and name H2' )( resid 9 and name H8 ) 2.60 0.44 0.44
assign ( resid 10 and name H2' )( resid 10 and name H8 ) 2.47 0.34 0.35
assign ( resid 11 and name H2' )( resid 11 and name H8 ) 2.73 0.56 0.56
assign ( resid 12 and name H2' )( resid 13 and name H6 ) 2.42 1.10 1.10
assign ( resid 13 and name H2' )( resid 13 and name H6 ) 2.19 0.32 0.32
assign ( resid 14 and name H2' )( resid 14 and name H6 ) 2.42 0.54 0.54
assign ( resid 16 and name H2' )( resid 16 and name H6 ) 2.42 0.49 0.49
assign ( resid 17 and name H2' )( resid 17 and name H6 ) 2.46 0.56 0.56
assign ( resid 18 and name H2' )( resid 18 and name H8 ) 2.78 0.59 0.59
assign ( resid 1 and name H2" )( resid 1 and name H6 ) 2.46 0.96 0.96
assign ( resid 3 and name H2" )( resid 3 and name H8 ) 3.12 0.69 0.69
assign ( resid 4 and name H2" )( resid 4 and name H8 ) 3.50 0.93 0.93
assign ( resid 10 and name H2" )( resid 10 and name H8 ) 3.00 0.67 0.67
assign ( resid 13 and name H2" )( resid 13 and name H6 ) 3.30 0.62 0.62
assign ( resid 15 and name H2" )( resid 15 and name H6 ) 3.40 0.54 0.54
assign ( resid 19 and name H2" )( resid 19 and name H6 ) 3.43 0.96 0.96
assign ( resid 4 and name H3' )( resid 4 and name H8 ) 3.30 1.05 1.05
assign ( resid 7 and name H3' )( resid 7 and name H8 ) 3.41 0.97 0.97
assign ( resid 9 and name H3' )( resid 9 and name H8 ) 3.42 0.98 0.99
assign ( resid 10 and name H3' )( resid 10 and name H8 ) 3.15 1.20 1.20
assign ( resid 14 and name H3' )( resid 14 and name H6 ) 2.60 1.40 1.40
assign ( resid 17 and name H3' )( resid 17 and name H6 ) 2.84 1.11 1.11
assign ( resid 18 and name H3' )( resid 18 and name H8 ) 3.29 1.08 1.08
assign ( resid 19 and name H3' )( resid 19 and name H6 ) 3.50 0.60 0.60
assign ( resid 21 and name H3' )( resid 21 and name H6 ) 4.20 0.58 0.57
assign ( resid 4 and name H8 )( resid 3 and name H3' ) 4.64 0.67 0.67
assign ( resid 7 and name H8 )( resid 6 and name H3' ) 4.12 0.79 0.79
assign ( resid 9 and name H8 )( resid 8 and name H3' ) 3.38 1.54 1.54
assign ( resid 10 and name H8 )( resid 9 and name H3' ) 4.75 0.76 0.76
assign ( resid 14 and name H6 )( resid 13 and name H3' ) 4.71 0.86 0.86
assign ( resid 16 and name H6 )( resid 15 and name H3' ) 3.72 1.03 1.04
assign ( resid 17 and name H6 )( resid 16 and name H3' ) 4.53 0.86 0.85
assign ( resid 18 and name H8 )( resid 17 and name H3' ) 5.04 0.85 0.85
assign ( resid 19 and name H6 )( resid 18 and name H3' ) 4.00 0.90 0.89
assign ( resid 9 and name H4' )( resid 9 and name H8 ) 4.75 0.94 0.93
assign ( resid 10 and name H4' )( resid 10 and name H8 ) 5.21 0.99 0.99
assign ( resid 17 and name H4' )( resid 17 and name H6 ) 3.16 1.43 1.42

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assign ( resid 3 and name H4' )( resid 4 and name H8 ) 5.75 0.92 0.92
assign ( resid 9 and name H4' )( resid 10 and name H8 ) 5.54 1.16 1.16
assign ( resid 17 and name H5' )( resid 17 and name H6 ) 3.46 0.89 0.88
assign ( resid 14 and name H5# )( resid 13 and name H2' ) 3.05 0.51 0.52
assign ( resid 9 and name H2 )( resid 9 and name H1' ) 4.54 0.45 0.45
assign ( resid 4 and name H2' )( resid 4 and name H1' ) 2.94 0.54 0.54
assign ( resid 9 and name H2' )( resid 9 and name H1' ) 2.66 0.32 0.32
assign ( resid 10 and name H2' )( resid 10 and name H1' ) 3.28 0.64 0.63
assign ( resid 18 and name H2' )( resid 18 and name H1' ) 2.75 0.50 0.50
assign ( resid 22 and name H2' )( resid 22 and name H1' ) 2.78 0.47 0.47
assign ( resid 7 and name H2'' )( resid 7 and name H1' ) 2.22 0.23 0.23
assign ( resid 10 and name H2'' )( resid 10 and name H1' ) 2.31 0.24 0.24
assign ( resid 13 and name H2'' )( resid 13 and name H1' ) 2.08 0.21 0.21
assign ( resid 14 and name H2'' )( resid 14 and name H1' ) 2.08 0.23 0.22
assign ( resid 19 and name H2'' )( resid 19 and name H1' ) 2.45 0.25 0.24
assign ( resid 14 and name H3' )( resid 14 and name H1' ) 3.33 0.76 0.76
assign ( resid 16 and name H3' )( resid 16 and name H1' ) 3.62 0.60 0.60
assign ( resid 7 and name H4' )( resid 7 and name H1' ) 3.17 0.51 0.52
assign ( resid 10 and name H4' )( resid 10 and name H1' ) 3.15 0.54 0.54
assign ( resid 14 and name H4' )( resid 14 and name H1' ) 2.81 0.90 0.90
assign ( resid 16 and name H4' )( resid 16 and name H1' ) 2.84 0.85 0.85
assign ( resid 17 and name H4' )( resid 17 and name H1' ) 3.04 0.64 0.64
assign ( resid 15 and name H4' )( resid 15 and name H1' ) 2.50 0.70 0.70
!assign ( resid 17 and name H5' )( resid 17 and name H1' ) 2.61 1.89 1.89
assign ( resid 2 and name H3' )( resid 2 and name H2' ) 2.31 0.30 0.30
assign ( resid 3 and name H3' )( resid 3 and name H2' ) 2.58 0.31 0.30
assign ( resid 6 and name H3' )( resid 6 and name H2' ) 2.51 0.31 0.31
assign ( resid 9 and name H3' )( resid 9 and name H2' ) 2.51 0.25 0.26
assign ( resid 10 and name H3' )( resid 10 and name H2' ) 2.27 0.25 0.25
assign ( resid 12 and name H3' )( resid 12 and name H2' ) 2.42 0.47 0.48
assign ( resid 14 and name H3' )( resid 14 and name H2' ) 2.01 0.47 0.47
assign ( resid 17 and name H3' )( resid 17 and name H2' ) 2.06 0.39 0.39
assign ( resid 1 and name H3' )( resid 1 and name H2'' ) 2.66 0.45 0.45
assign ( resid 2 and name H3' )( resid 2 and name H2'' ) 2.58 0.44 0.44
assign ( resid 3 and name H3' )( resid 3 and name H2'' ) 2.77 0.39 0.39
assign ( resid 6 and name H3' )( resid 6 and name H2'' ) 2.76 0.40 0.40
assign ( resid 9 and name H3' )( resid 9 and name H2'' ) 2.56 0.31 0.31
assign ( resid 10 and name H3' )( resid 10 and name H2'' ) 2.62 0.48 0.48
assign ( resid 12 and name H2' )( resid 13 and name H5' ) 2.46 1.34 1.34
assign ( resid 12 and name H2'' )( resid 12 and name H4' ) 2.65 1.44 1.44
assign ( resid 1 and name H2'' )( resid 1 and name H2' ) 1.99 0.20 0.20
assign ( resid 5 and name H2'' )( resid 5 and name H2' ) 2.12 0.32 0.32
assign ( resid 9 and name H2'' )( resid 9 and name H2' ) 1.89 0.19 0.19
assign ( resid 19 and name H2'' )( resid 19 and name H2' ) 1.86 0.19 0.19
assign ( resid 22 and name H2'' )( resid 22 and name H2' ) 2.09 0.27 0.27
assign ( resid 2 and name H3' )( resid 2 and name H4' ) 2.43 0.33 0.33

```

```
assign ( resid 8 and name H4' )( resid 8 and name H3' ) 2.65 0.36 0.36  
assign ( resid 8 and name H5' )( resid 8 and name H3' ) 2.05 1.76 1.76
```

```
set message=on echo=on end
```

Figure S1. Partial charges on β -styrene adduct

