

*t**t*

fn \rightarrow *fn_new*

fn \rightarrow *fn_new*

fn_new → *fn_ql*

fn_new → *fn_ql*

	F 0	1 STATES		F 0	1 STATES		F 0	1 STATES	
	1S			1S			1S		
	CFP FOR F 0	1 STATES	1 PARENTS	CFP FOR F 0	1 STATES	1 PARENTS	CFP FOR F 0	1 STATES	1 PARENTS
	... 6 6 6 ...		
	V (1K) FOR F 0	1 STATES		V (1K) FOR F 0	1 STATES		V (1K) FOR F 0	1 STATES	
	1S 1S	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
	END			END			END		

flcross:

fn

fn -> fn_new

fn_new -> fn_ql

.	F 1 1 STATES	F 1 1 STATES	F 1 1 STATES
.	2F	2F	2F
.	CFP FOR F 0 1 STATES 1 PARENTS	CFP FOR F 0 1 STATES 1 PARENTS	CFP FOR F 0 1 STATES 1 PARENTS
.	... 6 6 6 ...
.	V (1K) FOR F 1 1 STATES	V (1K) FOR F 1 1 STATES	V (1K) FOR F 1 1 STATES
.	2F 2F 1.224745 1.224745 1.224745 1.224745 1.224745 1.224745 1.224745	2F 2F 1.224745 1.224745 1.224745 1.224745 1.224745 1.224745 1.224745	2F 2F 1.224745 1.224745 1.224745 1.224745 1.224745 1.224745 1.224745
.	END	END	END

*f**f*
$$fn \rightarrow fn_new$$

fn_new → *fn_ql*

	F 2 7 STATES								F 2 7 STATES								F 2 7 STATES																			
	3P	3F	3H	1S	1D	1G	1I		3P	3F	3H	1S	1D	1G	1I		3P	3F	3H	1S	1D	1G	1I													
	CFP FOR F 2				7 STATES				1 PARENTS				CFP FOR F 2				7 STATES				1 PARENTS				CFP FOR F 2				7 STATES				1 PARENTS			
	... 68 68 68 ...																			
	3F	1G	-38.141184		8.090556		-10.575741	-0.165831	0.156085	-0.030749		3F	1G	-38.141184		8.090556		-10.575741	-0.165831	0.156085	-0.030749		3F	1G	-38.141184		8.090556		-10.575741	-0.165831	0.156085	-0.030749				
	3H	3H	-101.601915		21.102453		11.063005	0.535614	0.216221	-0.022919		3H	3H	-101.601915		21.102453		11.063005	0.535614	0.216221	-0.022919		3H	3H	-101.601915		21.102453		11.063005	0.535614	0.216221	-0.022919				
	3H	1G	42.058291		-15.533488		-6.250511	0.263523	-0.122687	-0.029318		3H	1G	42.058291		-15.533488		-6.250511	0.263523	-0.122687	-0.029318		3H	1G	42.058291		-15.533488		-6.250511	0.263523	-0.122687	-0.029318				
	3H	1I	-41.004614		0.708200		-8.031265	-0.214820	0.166612	-0.035657		3H	1I	-39.517403		-12.631662		-0.636162	0.099148	-0.004097	0.01030		3H	1I	-39.517403		-12.631662		-0.636162	0.099148	-0.004097	0.01030				
	END								END								END																			

f3cross:

fn

fn -> fn_new

fn_new -> fn_ql

	F 3 17 STATES																		F 3 17 STATES																		F 3 17 STATES																															
	4S	4D	4F	4G	4I	2P	2D1	2D2	2F1	2F2	2G1	2G2	2H1	2H2	2I	2K	2L		4S	4D	4F	4G	4I	2P	2D1	2D2	2F1	2F2	2G1	2G2	2H1	2H2	2I	2K	2L		4S	4D	4F	4G	4I	2P	2D1	2D2	2F1	2F2	2G1	2G2	2H1	2H2	2I	2K	2L															
	CFP FOR F 3				17 STATES				7 PARENTS									CFP FOR F 3				17 STATES				7 PARENTS									CFP FOR F 3				17 STATES				7 PARENTS									CFP FOR F 3				17 STATES				7 PARENTS								
	... 326 326 326 ...																															
	4D	2D1	-2.948230		-29.641666		-9.235855		0.535639		-0.233412		0.027087					4D	2D1	-2.948230		-29.641666		-9.235855		0.535639		-0.233412		0.027087					4D	2D1	-2.948230		-29.641666		-9.235855		0.535639		-0.233412		0.027087																					
	4D	2D2	33.872588		-19.668846		-26.115004		-0.457738		0.077761		0.084874					4D	2D2	33.872588		-19.668846		-26.115004		-0.457738		0.077761		0.084874					4D	2D2	33.872588		-19.668846		-26.115004		-0.457738		0.077761		0.084874																					
	4D	2F1	-20.448307		11.197882		12.392909		0.973729		0.405720		-0.000000					4D	2F1	-20.448307		11.197882		12.392909		0.973729		0.405720		-0.000000					4D	2F1	-20.448307		11.197882		12.392909		0.973729		0.405720		-0.000000																					
●																																																																				
	4F	4F	-151.846040		-3.944053		6.274629		0.284848		0.159356		0.134073					4F	4F	-151.846040		-3.944053		6.274629		0.284848		0.159356		0.134073					4F	4F	-151.846040		-3.944053		6.274629		0.284848		0.159356		0.134073																					
	4F	4G	38.535695		49.823924		38.040283		0.333024		0.082568		-0.185249					4F	4G	38.535695		49.823924		38.040283		0.333024		0.082568		-0.185249					4F	4G	38.535695		49.823924		38.040283		0.333024		0.082568		-0.185249																					
	4F	2D1	23.186202		-20.977988		-14.052246		0.000000		-0.000000		-0.000000					4F	2D1	23.186202		-20.977988		-14.052246		0.000000		-0.000000		-0.000000					4F	2D1	23.186202		-20.977988		-14.052246		0.000000		-0.000000		-0.000000																					
	... 11 11 11 ...																															
	4G	2H2	-39.572828		-10.928856		-15.147899		0.439698		-0.026841		-0.124004					4G	2H2	-39.572828		-10.928856		-15.147899		0.439698		-0.026841		-0.124004					4G	2H2	-39.572828		-10.928856		-15.147899		0.439698		-0.026841		-0.124004																					
	4I	4I	-311.717449		39.307475		30.332407		1.228993		0.530932		0.062149					4I	4I	-311.717449		39.307475		30.332407		1.228993		0.530932		0.062149					4I	4I	-311.717449		39.307475		30.332407		1.228993		0.530932		0.062149																					
	4I	2H1	18.696404		-19.675002		1.067921		0.396590		-0.207582		0.050910					4I	2H1	18.696404		-19.675002		1.067921		0.396590		-0.207582		0.050910					4I	2H1	18.696404		-19.675002		1.067921		0.396590		-0.207582		0.050910																					
●	4I	2I	-61.355065		13.961230		17.395113		-0.409034		-0.033292		0.167067					4I	2H2	-61.355065		13.961230		17.395113		-0.409034		-0.033292		0.167067					4I	2H2	-61.355065		13.961230		17.395113		-0.409034		-0.033292		0.167067																					
●	4I	2K	-49.290519		-16.687699		4.230274		-0.207738		-0.040580		0.105860					4I	2I	-49.290519		-16.687699		4.230274		-0.207738		-0.040580		0.105860					4I	2I	-49.290519		-16.687699		4.230274		-0.207738		-0.040580		0.105860																					
●	4I	2L	70.230096		17.181956		15.206329		0.229510		-0.092468		0.004910					4I	2K	70.230096		17.181956		15.206329		0.229510		-0.092468		0.004910					4I	2K	70.230096		17.181956		15.206329		0.229510		-0.092468		0.004910																					
●																																																																				
	2P	2P	-13.999999		-9.000003		19.090912		0.288889		-0.227273		0.135975					2P	2P	-13.999999		-9.000003		19.090912		0.288889		-0.227273		0.135975					2P	2P	-13.999999		-9.000003		19.090912		0.288889		-0.227273		0.135975																					
	2P	2D1	-13.955371		9.954180		-2.528468		0.059638		0.014786		-0.033175					2P	2D1	-13.955371		9.954180		-2.528468		0.059638		0.014786		-0.033175					2P	2D1	-13.955371		9.954180		-2.528468		0.059638		0.014786		-0.033175																					
	2P	2D2	3.363671		-3.771386		-12.138873		0.186871		0.046332		-0.103949					2P	2D2	3.363671		-3.771386		-12.138873		0.186871		0.046332		-0.103949					2P	2D2	3.363671		-3.771386		-12.138873		0.186871		0.046332		-0.103949																					
	... 29 29 29 ...																															
	2K	2L	-68.224626		-7.738828		2.299513		-0.307318		0.057146		0.052600					2K	2L	-68.224626		-7.738828		2.299513		-0.307318		0.057146		0.052600					2K	2L	-68.224626		-7.738828		2.299513		-0.307318		0.057146		0.052600																					
	2L	2L	-149.969990		16.555128		12.870911		0.714143		0.257393		-0.020372					2L	2L	-149.969990		16.555128		12.870911		0.714143		0.257393		-0.020372					2L	2L	-149.969990		16.555128		12.870911		0.714143		0.257393		-0.020372																					
	END																		END																		END																															

fm

fn → *fn_new*

fn_new → *fn_ql*

	F 4 47 STATES																			F 4 47 STATES																			F 4 47 STATES																					
	5S	5D	5F	5G	5I	3P1	3P2	3P3	3D1	3D2	3F1	3F2	3F3	3F4	3G1	3G2	3G3	3H1	3H2	3H3	5S	5D	5F	5G	5I	3P1	3P2	3P3	3D1	3D2	3F1	3F2	3F3	3F4	3G1	3G2	3G3	3H1	3H2	3H3	5S	5D	5F	5G	5I	3P1	3P2	3P3	3D1	3D2	3F1	3F2	3F3	3F4	3G1	3G2	3G3	3H1	3H2	3H3
	3H4	3I1	3I2	3K1	3K2	3L	3M	1S1	1S2	1D1	1D2	1D3	1D4	1F	1G1	1G2	1G3	1G4	1H1	1H2	3H4	3I1	3I2	3K1	3K2	3L	3M	1S1	1S2	1D1	1D2	1D3	1D4	1F	1G1	1G2	1G3	1G4	1H1	1H2	3H4	3I1	3I2	3K1	3K2	3L	3M	1S1	1S2	1D1	1D2	1D3	1D4	1F	1G1	1G2	1G3	1G4	1H1	1H2
	... 1520 1520 1520 ...																					
	3P1	3D2	-4.254745			-19.081886			-21.156506			-0.236375			-0.058605			0.131486			3P1	3D2	-4.254745			-19.081886			-21.156506			-0.236375			-0.058605			0.131486			3P1	3D2	-4.254745			-19.081886			-21.156506			-0.236375			-0.058605			0.131486		
	3P1	1S1	13.168142			0.774597			0.352089			-0.421725			-0.191693			-0.052663			3P1	1S1	13.168142			0.774597			0.352089			-0.421725			-0.191693			-0.052663			3P1	1S1	13.168142			0.774597			0.352089			-0.421725			-0.191693			-0.052663		
	3P1	1S2	9.082950			6.440637			5.930189			-0.100922			-0.065891			-0.078594			3P1	1S2	9.082950			6.440637			5.930189			-0.100922			-0.065891			-0.078594			3P1	1S2	9.082950			6.440637			5.930189			-0.100922			-0.065891			-0.078594		
●	3P1	1D1	-14.405093			-7.832433			-6.249016			-0.088244			-0.278011			-0.093096			3P1	1D1	-14.405093			-7.832433			-6.249016			-0.088244			-0.278011			-0.093096			3P1	1D1	-14.405093			-7.832433			-6.249016			-0.088244			-0.278011			-0.093096		
	3P1	1D2	-5.396457			-4.002023			-0.373962			-0.211489			-0.066552			0.071103			3P1	1D2	-5.396457			-4.002023			-0.373962			-0.211489			-0.066552			0.071103			3P1	1D2	-5.396457			-4.002023			-0.373962			-0.211489			-0.066552			0.071103		
	3P1	1D4	-15.378108			0.155334			2.612441			0.366145			0.173154			0.067891			3P1	1D4	-15.378108			0.155334			2.612441			0.366145			0.173154			0.067891			3P1	1D4	-15.378108			0.155334			2.612441			0.366145			0.173154			0.067891		
	3P2	3P2	-24.066665			10.299993			35.454548			0.261481			-0.175253			0.131443			3P2	3P2	-24.066665			10.299993			35.454548			0.261481			-0.175253			0.131443			3P2	3P2	-24.066665			10.299993			35.454548			0.261481			-0.175253			0.131443		
	... 227 227 227 ...																					
	3M	1L2	65.909278			10.107972			-11.091995			0.468607			0.120291			-0.178379			3M	1L2	65.909278			10.107972			-11.091995			0.468607			0.120291			-0.178379			3M	1L2	65.909278			10.107972			-11.091995			0.468607			0.120291			-0.178379		
	3M	1N	55.637890			7.720087			10.881103			0.534533			-0.102758			-0.022872			3M	1N	55.637890			7.720087			10.881103			0.534533			-0.102758			-0.022872			3M	1N	55.637890			7.720087			10.881103			0.534533			-0.102758			-0.022872		
	END																			END																			END																					

fn	fn -> fn_new																											fn_new -> fn_gl																													
	F 5													73 STATES															F 5													73 STATES															
6P 6F 6H 4S 4P1 4P2 4D1 4D2 4D3 4F1 4F2 4F3 4F4 4G1 4G2 4G3 4G4 4H1 4H2 4H3																																																									
4I1 4I2 4I3 4K1 4K2 4L 4M 2P1 2P2 2P3 2P4 2D1 2D2 2D3 2D4 2D5 2F1 2F2 2F3 2F4																																																									
... 4099 ...																																																									
6P 4P2	23.073793 -5.688992 -7.223201 -0.116534 0.156503 0.064824																												6P 4P2	23.073793 -5.688992 -7.223201 -0.116534 0.156503 0.064824																											
6P 4D1	15.336230 -8.398412 -9.294682 -0.730297 -0.304290 0.000000																												6P 4D1	15.336230 -8.398412 -9.294682 -0.730297 -0.304290 0.000000																											
6P 4D2	17.389650 -0.552052 -4.391325 -0.000000 -0.000000 0.000000																												6P 4D2	17.389650 -0.552052 -4.391325 -0.000000 -0.000000 0.000000																											
●	6P 4D3 0.000006 -37.713890 -57.729126 0.000000 0.000000 0.000000																												6P 4D3	0.000006 -37.713890 -57.729126 0.000000 0.000000 0.000000																											
	6F 6F	-247.922557 26.563131 0.000001 1.180583 0.491910 0.000000																											6F 6F	-247.922557 26.563131 0.000001 1.180583 0.491910 0.000000																											
	6F 4D1	23.400852 14.968113 10.253442 -0.035136 -0.079855 -0.214996																											6F 4D1	23.400852 14.968113 10.253442 -0.035136 -0.079855 -0.214996																											
6F 4D2	16.016062 -34.980349 -40.673989 0.013280 0.030182 0.081261																											6F 4D2	16.016062 -34.980349 -40.673989 0.013280 0.030182 0.081261																												
... 3 ...																																																									
6F 4F3	-0.000001 15.045161 -10.746542 -0.225166 -0.023261 -0.062626																											6F 4F3	-0.000001 15.045161 -10.746542 -0.225166 -0.023261 -0.062626																												
6F 4F4	18.865606 84.609373 56.448890 0.000000 0.303166 -0.269083																											6F 4F4	18.865606 84.609373 56.448890 0.000000 0.303166 -0.269083																												
6F 4G1	-19.899747 5.125692 12.334549 0.294811 0.147710 0.081996																											6F 4G1	-19.899747 5.125692 12.334549 0.294811 0.147710 0.081996																												
●	6F 4G2 -32.592720 -34.150185 -35.880318 -0.111428 -0.055829 -0.030992																												6F 4G2	-32.592720 -34.150185 -35.880318 -0.111428 -0.055829 -0.030992																											
	6F 4G3	1.407465 -3.049503 -13.393860 -0.281493 0.231023 0.055206																											6F 4G3	1.407465 -3.049503 -13.393860 -0.281493 0.231023 0.055206																											
	6F 4G4	9.062745 -40.645028 -32.705765 0.604183 -0.228857 0.000000																											6F 4G4	9.062745 -40.645028 -32.705765 0.604183 -0.228857 0.000000																											
6H 6H	-586.167591 5.743615 0.870246 1.754993 0.829955 0.325412																											6H 6H	-586.167591 5.743615 0.870246 1.754993 0.829955 0.325412																												
... 123 ...																																																									
4F1 2F5	-4.084523 -18.318468 -20.310088 -0.226918 -0.056261 0.126226																											4F1 2F5	-4.084523 -18.318468 -20.310088 -0.226918 -0.056261 0.126226																												
4F1 2F6	-0.788811 -3.537696 -3.922321 -0.043823 -0.010865 0.024377																											4F1 2F6	-0.788811 -3.537696 -3.922321 -0.043823 -0.010865 0.024377																												
4F1 2F7	2.358200 10.576172 11.726035 0.131011 0.032482 -0.072877																											4F1 2F7	2.358200 10.576172 11.726035 0.131011 0.032482 -0.072877																												
●	4F1 2G1 -13.027446 -15.681176 -26.537392 -0.771997 -0.337948 -0.053679																												4F1 2G1	-13.027446 -15.681176 -26.537392 -0.771997 -0.337948 -0.053679																											
	4F1 2G2	-4.093984 -28.083300 9.188988 0.667966 -0.081619 0.152129																											4F1 2G2	-4.093984 -28.083300 9.188988 0.667966 -0.081619 0.152129																											
	4F1 2G3	0.000000 -6.733038 -6.978272 -0.176916 -0.060146 0.044733																											4F1 2G3	0.000000 -6.733038 -6.978272 -0.176916 -0.060146 0.044733																											
4F1 2G4	-5.002499 10.806264 9.577784 0.595536 0.228042 -0.066255																											4F1 2G4	-5.002499 10.806264 9.577784 0.595536 0.228042 -0.066255																												
... 92 ...																																																									
4G1 2G5	5.732461 8.578647 5.375319 0.298872 0.093942 -0.100841																											4G1 2G5	5.732461 8.578647 5.375319 0.298872 0.093942 -0.100841																												
4G1 2G6	-15.503869 -1.464072 0.779712 0.340524 0.165544 0.077997																											4G1 2G6	-15.503869 -1.464072 0.779712 0.340524 0.165544 0.077997																												
●	4G1 2H1 -24.244128 -31.769707 -5.014923 -0.227215 -0.374111 0.110755																												4G1 2H1	-24.244128 -31.769707 -5.014923 -0.227215 -0.374111 0.110755																											
	4G1 2H2 -19.336720 -25.986700 -33.327564 -0.484667 -0.407778 -0.110107																												4G1 2H2	-19.336720 -25.986700 -33.327564 -0.484667 -0.407778 -0.110107																											
	4G1 2H3	-8.198915 -3.395510 1.392836 -0.184959 -0.051447 0.084458																											4G1 2H3	-8.198915 -3.395510 1.392836 -0.184959 -0.051447 0.084458																											
4G1 2H4	5.559067 -3.137675 -6.958013 0.012554 -0.001971 -0.023744																											4G1 2H4	5.559067 -3.137675 -6.958013 0.012554 -0.001971 -0.023744																												
4G1 2H5	1.471960 -2.929052 -5.548571 0.070872 0.028610 -0.003033																											4G1 2H5	1.471960 -2.929052 -5.548571 0.070872 0.028610 -0.003033																												
... 141 ...																																																									
4H3 2I1	7.889749 -3.381321 -10.758744 0.205742 0.069123 -0.054735																											4H3 2I1	7.889749 -3.381321 -10.758744 0.205742 0.069123 -0.054735																												
4H3 2I2	10.465994 -5.596499 -21.474674 -0.094820 0.084648 -0.017990																											4H3 2I2	10.465994 -5.596499 -21.474674 -0.094820 0.084648 -0.017990																												
4H3 2I3	-12.549900 9.172274 -16.626132 -0.724072 0.262070 0.010828																											4H3 2I3	-12.549900 9.172274 -16.626132 -0.724072 0.262070 0.010828																												
●	4H3 2I4 -39.062313 -34.720749 -41.006706 -0.257267 -0.061508 -0.000383																												4H3 2I4	-39.062313 -34.720749 -41.006706 -0.257267 -0.061508 -0.000383																											
	4H3 2I5	3.192166 -66.745280 -86.459220 -0.060505 0.016381 0.064724																											4H3 2I5	3.192166 -66.745280 -86.459220 -0.060505 0.016381 0.064724																											
	4I1 4I1	-367.022154 27.880883 20.983380 2.737303 1.244229 0.341821																											4I1 4I1	-367.022154 27.880883 20.983380 2.737303 1.244229 0.341821																											
4I1 4I2	5.700877 6.852569 1.230217 0.443401 0.152686 -0.105706																											4I1 4I2	5.700877 6.852569 1.230217 0.443401 0.152686 -0.105706																												
... 112 ...																																																									
2P1 2P2	-0.707107 -7.621039 -8.606700 -0.117851 -0.034522 0.048074																											2P1 2P2	-0.707107 -7.621039 -8.606700 -0.117851 -0.034522 0.048074																												
2P1 2P3	-10.382677 0.104875 1.763815 0.247207 0.116907 0.045837																											2P1 2P3	-10.382677 0.104875 1.763815 0.247207 0.116907 0.045837																												
2P1 2D1	4.440343 12.084895 -1.293807 -0.474396 -0.232885 -0.116111																											2P1 2D1	4.440343 12.084895 -1.293807 -0.474396 -0.232885 -0.116111																												
●	2P1 2D2 0.000000 -18.856945 -28.864569 0.000000 0.000000 0.000000																												2P1 2D2	0.000000 -18.856945 -28.864569 0.000000 0.000000 0.000000																											
	2P1 2D3	-2.878905 2.976495 2.151415 0.257529 0.102272 -0.016587																											2P1 2D3	-2.878905 2.976495 2.151415 0.257529 0.102272 -0.016587																											
	2P1 2D4	3.718678 16.677709 18.490942 0.206593 0.051221 -0.114920																											2P1 2D4	3.718678 16.677709 18.490942 0.206593 0.051221 -0.114920																											
2P2 2P2	-10.222222 40.462956 24.023567 -0.244444 0.165264 -0.045325																											2P2 2P2	-10.222222 40.462956 24.023567 -0.244444 0.165264 -0.045325																												
... 111 ...																																																									
2F4 2G2	0.287297 1.288484 1.428571 0.015961 0.003957 -0.008878																											2F4 2G2	0.287297 1.288484 1.428571 0.015961 0.003957 -0.008878																												
2F4 2G3	4.600179 -5.305651 9.624960 0.363640 -0.123754 0.015284																											2F4 2G3	4.600179 -5.305651 9.624960 0.363640 -0.123754 0.015284																												
2F4 2G4	10.726860 44.806146 40.473320 0.059834 0.078218 -0.089541																											2F4 2G4	10.726860 44.806146 40.473320 0.059834 0.078218 -0.089541																												
●	2F4 2G5 -11.034564 -19.813456 -30.896538 -0.090124 -0.024718 -0.020059																												2F4 2G5	-11.034564 -19.813456 -30.896538 -0.090124 -0.024718 -0.020059																											
	2F4 2G6	-17.562978 -29.606794 2.057207 0.232958 -0.208199 0.116006																											2F4 2G6	-17.562978 -29.606794 2.057207 0.232958 -0.208199 0.116006																											
	2F5 2F5	-42.325765 -5.274643 -6.350759 0.067019 0.073648 0.065384																											2F5 2F5	-42.325765 -5.274643 -6.350759 0.067019 0.073648 0.065384																											
2F5 2F6	-0.078281 -47.530912 -39.491358 0.216578 -0.165272 0.08615																																																								

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F 11 17 STATES																	F 11 17 STATES																	F 11 17 STATES																										
4S	4D	4F	4G	4I	2P	2D1	2D2	2F1	2F2	2G1	2G2	2H1	2H2	2I	2K	2L	4S	4D	4F	4G	4I	2P	2D1	2D2	2F1	2F2	2G1	2G2	2H1	2H2	2I	2K	2L	4S	4D	4F	4G	4I	2P	2D1	2D2	2F1	2F2	2G1	2G2	2H1	2H2	2I	2K	2L										
CFP FOR F 11 47 STATES 17 PARENTS																	CFP FOR F 11 47 STATES 17 PARENTS																	CFP FOR F 11 47 STATES 17 PARENTS																										
... 380 380 380 ...																										
-0.075400 11007008 0.044087 11011012 -0.452267 11013014																	-0.075400 11007008 0.044087 11011012 -0.452267 11013014																	-0.075400 11007008 0.044087 11011012 -0.452267 11013014																										
END																	END																	END																										
MK,PK FOR F 11 17 STATES																	MK,PK FOR F 11 17 STATES																	MK,PK FOR F 11 17 STATES																										
4S	2P	11.313709			-7.542472			1.714198			0.0			0.0			0.0			4S	2P	11.313709			-7.542472			1.714198			0.000000			-0.000000			0.000000			4S	2P	11.313709			-7.542472			1.714198			0.000000			-0.000000			0.000000			
4D	4D	-56.097135			85.324201			91.495317			0.602350			0.202371			-0.160248			4D	4D	-56.097135			85.324201			91.495317			0.602350			0.202371			-0.160248			4D	4D	-56.097135			85.324201			91.495317			0.602350			0.202371			-0.160248			
4D	4F	19.595916			-29.393869			-48.989786			0.0			0.0			0.0			4D	4F	19.595916			-29.393869			-48.989786			-0.000000			-0.000000			0.000000			4D	4F	19.595916			-29.393869			-48.989786			-0.000000			-0.000000			0.000000			
4D	2P	8.398412			-8.033263			2.821599			-0.223146			-0.055326			0.124128			4D	2P	8.398412			-8.033263			2.821599			-0.223146			-0.055326			0.124128			4D	2P	8.398412			-8.033263			2.821599			-0.223146			-0.055326			0.124128			
4D	2D1	-2.948230			-29.641666			-9.235855			0.535639			-0.233412			0.027087			4D	2D1	-2.948230			-29.641666			-9.235855			0.535639			-0.233412			0.027087			4D	2D1	-2.948230			-29.641666			-9.235855			0.535639			-0.233412			0.027087			
4D	2D2	33.872588			-19.668846			-26.115004			-0.457738			0.077761			0.084874			4D	2D2	33.872588			-19.668846			-26.115004			-0.457738			0.077761			0.084874			4D	2D2	33.872588			-19.668846			-26.115004			-0.457738			0.077761			0.084874			
4D	2F1	-20.448307			11.197882			12.392909			0.973729			0.405720			0.0			4D	2F1	-20.448307			11.197882			12.392909			0.973729			0.405720			-0.000000			4D	2F1	-20.448307			11.197882			12.392909			0.973729			0.405720			-0.000000			
																				4D	2F2	-0.000002			-38.405949			-58.788467			0.000000			0.000000			0.000000			4D	2F2	-0.000002			-38.405949			-58.788467			0.000000			0.000000			0.000000			
	4F	4F	-151.846040			-3.944053			6.274629			0.284848			0.159356			0.134073			4F	4F	-151.846040			-3.944053			6.274629			0.284848			0.159356			0.134073			4F	4F	-151.846040			-3.944053			6.274629			0.284848			0.159356			0.134073		
	4F	4G	38.535695			49.823924			38.040283			0.333024			0.082568			-0.185249			4F	4G	38.535695			49.823924			38.040283			0.333024			0.082568			-0.185249			4F	4G	38.535695			49.823924			38.040283			0.333024			0.082568			-0.185249		
	4F	2D1	23.186202			-20.977988			-14.052246			0.0			0.0			0.0			4F	2D1	23.186202			-20.977988			-14.052246			0.000000			-0.000000			-0.000000			4F	2D1	23.186202			-20.977988			-14.052246			0.000000			-0.000000			-0.000000		
	4F	2D2	-7.399699			-28.902071			-5.503906			0.411094			-0.284538			0.114338			4F	2D2	-7.399699			-28.902071			-5.503906			0.411094			-0.284538			0.114338			4F	2D2	-7.399699			-28.902071			-5.503906			0.411094			-0.284538			0.114338		
	4F	2F1	-19.402174			-3.527668			0.801742			0.254776			0.142532			0.119919			4F	2F1	-19.402174			-3.527668			0.801742			0.254776			0.142532			0.119919			4F	2F1	-19.402174			-3.527668			0.801742			0.254776			0.142532			0.119919		
	4F	2F2	-22.751068			-11.845597			-0.256397			-0.114904			-0.114904			0.140617			4F	2F2	-22.751068			-11.845597			-0.256397			-0.114904			-0.114904			0.140617			4F	2F2	-22.751068			-11.845597			-0.256397			-0.114904			-0.114904			0.140617		
... 8 8 8 ...																										
	4G	2H2	-39.572828			-10.928856			-15.147899			0.439698			-0.026841			-0.124004			4G	2H2	-39.572828			-10.928856			-15.147899			0.439698			-0.026841			-0.124004			4G	2H2	-39.572828			-10.928856			-15.147899			0.439698			-0.026841			-0.124004		
	4I	4I	-311.717449			39.307475			30.332407			1.228993			0.530932			0.062149			4I	4I	-311.717449			39.307475			30.332407			1.228993			0.530932			0.062149			4I	4I	-311.717449			39.307475			30.332407			1.228993			0.530932			0.062149		
	4I	2H1	18.696404			-19.675002			1.067921			0.396590			-0.207582			0.050910			4I	2H1	18.696404			-19.675002			1.067921			0.396590			-0.207582			0.050910			4I	2H1	18.696404			-19.675002			1.067921			0.396590			-0.207582			0.050910		
	4I	2I	-61.355065			13.961230			17.395113			-0.409034			-0.033292			0.167067			4I	2H2	-61.355065			13.961230			17.395113			-0.409034			-0.033292			0.167067			4I	2H2	-61.355065			13.961230			17.395113			-0.409034			-0.033292			0.167067		
	4I	2K	-49.290519			-16.687699			4.230274			-0.207738			-0.040580			0.105860			4I	2I	-49.290519			-16.687699			4.230274			-0.207738			-0.040580			0.105860			4I	2I	-49.290519			-16.687699			4.230274			-0.207738			-0.040580			0.105860		
	4I	2L	70.230096			17.181956			15.206329			0.229510			-0.092468			0.004910			4I	2K	70.230096			17.181956			15.206329			0.229510			-0.092468			0.004910			4I	2K	70.230096			17.181956			15.206329			0.229510			-0.092468			0.004910		
																					4I	2L	0.000000			0.000000			0.000000			0.000000			0.000000			0.000000			4I	2L	0.000000			0.000000			0.000000			0.000000			0.000000					
	2P	2P	-13.999999			-9.000003			19.090912			0.288889			-0.227273			0.135975			2P	2P	-13.999999			-9.000003			19.090912			0.288889			-0.227273			0.135975			2P	2P	-13.999999			-9.000003			19.090912			0.288889			-0.227273			0.135975		
	2P	2D1	-13.955371			9.954180			-2.528468			0.059638			0.014786			-0.033175			2P	2D1	-13.955371			9.954180			-2.528468			0.059638			0.014786			-0.033175			2P	2D1	-13.955371			9.954180			-2.528468			0.059638			0.014786			-0.033175		
	2P	2D2	3.363671			-3.771386			-12.138873			0.186871			0.046332			-0.103949			2P	2D2	3.363671			-3.771386			-12.138873			0.186871			0.046332			-0.103949			2P	2D2	3.363671			-3.771386			-12.138873			0.186871			0.046332			-0.103949		
	2D1	2D1	-33.562314			9.859998			-12.041861			0.016090			0.236083			-0.144786			2D1	2D1	-33.562314			9.859998			-12.041861			0.016090			0.236083			-0.144786			2D1	2D1	-33.562314			9.859998			-12.041861			0.016090			0.236083			-0.144786		
	2D1	2D2	-20.307700			13.249307			17.234819			0.024467			-0.034825			0.022684			2D1	2D2	-20.307700			13.249307			17.234819			0.024467			-0.034825			0.022684			2D1	2D2	-20.307700			13.249307			17.234819			0.024467			-0.034825			0.022684		
	2D1	2F1	-0.780719			-4.033720			-8.398651			0.260240			0.108433			0.0			2D1	2F1	-0.780719			-4.033720			-8.398651			0.260240			0.108433			0.000000			2D1	2F1	-0.780719			-4.033720			-8.398651			0.260240			0.108433			0.000000		
	2D1	2F2	5.492852			29.766814			35.168881			0.0			0.0			0.0			2D1	2F2	5.492852			29.766814			35.168881			-0.000000			-0.000000			-0.000000			2D1	2F2	5.492852			29.766814			35.168881			-0.000000			-0.000000			-0.000000		
	2D2	2D2	-10.711830			40.769997			36.811079			-0.378830			0.168421			0.048042			2D2	2D2	-10.711830			40.769997			36.811079			-0.378830			0.168421			0.048042			2D2	2D2	-10.711830			40.769997			36.811079			-0.378830			0.168421			0.048042		
	2D2	2F1	-17.192097			-15.493273			-15.938051			0.207634			0.135563			0.161699			2D2	2F1	-17.192097			-15.493273			-15.938051			0.207634			0.135563			0.161699			2D2	2F1	-17.192097			-15.493273			-15.938051			0.207634			0.135563			0.161699		
	2D2	2F2	-18.486201			38.558791			48.750830			0.495799			0.006402			-0.172371			2D2	2F2	-18.486201			38.558791			48.750830			0.495799			0.006402			-0.172371			2D2	2F2	-18.486201			38.558791			48.750830			0.495799			0.006402			-0.172371		
	2F1	2F1	-21.202723			-1.247219			-0.566918			0.679041			0.308655			0.084795			2F1	2F1	-21.202723			-1.247219			-0.566918			0.679041			0.308655			0.084795			2F1	2F1	-21.202723			-1.247219			-0.566918			0.679041			0.308655			0.084795		
	2F1	2F2	23.399902			8.509056			7.493768			-0.519998			-0.260536			-0.144628			2F1	2F2	23.399902			8.509056			7.493768			-0.519998			-0.260536			-0.144628			2F1	2F2	23.399902			8.509056			7.493768			-0.519998			-0.260536			-0.144628		
	2F																																																											

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	F 12 7 STATES								F 12 7 STATES								F 12 7 STATES																			
	3P	3F	3H	1S	1D	1G	1I		3P	3F	3H	1S	1D	1G	1I		3P	3F	3H	1S	1D	1G	1I													
	CFP FOR F 12				17 STATES				7 PARENTS				CFP FOR F 12				17 STATES				7 PARENTS				CFP FOR F 12				17 STATES				7 PARENTS			
	... 72 72 72 ...																			
	3H	-0.909137			0.0		0.0		0.0		0.0		0.0		0.0		3H	-0.909137			0.0		0.0		0.0		0.0		0.0							
	1S	0.0			0.0		0.0		0.0		0.0		0.0		0.0		1S	0.0			0.0		0.0		0.0		0.0		0.0							
	1D	-1.111168			0.0		0.0		0.0		0.0		0.0		0.0		1D	-1.111168			0.0		0.0		0.0		0.0		0.0							
●	1G	0.0			0.0		0.0		0.0		0.0		0.0		0.0		1G	-0.404061			0.0		0.0		0.0		0.0		0.0							
	1I	0.707107			0.0		0.0		0.0		0.0		0.0		0.0		1I	0.707107			0.0		0.0		0.0		0.0		0.0							
	END								END								END																			
	MK,PK FOR F 12				7 STATES				MK,PK FOR F 12				7 STATES				MK,PK FOR F 12				7 STATES															
	... 5 5 5 ...																			
	3F	1G	-38.141184			8.090556		-10.575741		-0.165831		0.156085		-0.030749		3F	1G	-38.141184			8.090556		-10.575741		-0.165831		0.156085		-0.030749							
	3H	3H	-101.601915			21.102453		11.063005		0.535614		0.216221		-0.022919		3H	3H	-101.601915			21.102453		11.063005		0.535614		0.216221		-0.022919							
	3H	1G	42.058291			-15.533488		-6.250511		0.263523		-0.122687		-0.029318		3H	1G	42.058291			-15.533488		-6.250511		0.263523		-0.122687		-0.029318							
●	3H	1I	-41.004614			0.708200		-8.031265		-0.214820		0.166612		-0.035657		3H	1I	-39.517403			-12.631662		-0.636162		0.099148		-0.004097		0.01030							
	END								END								END																			

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fn → *fn_new*

fn → *fn_new*

fn_new → *fn_ql*

fn_new → *fn_ql*

F 13	1 STATES	F 13	1 STATES	F 13	1 STATES
2F		2F		2F	
CFP FOR F 13	7 STATES 1 PARENTS	CFP FOR F 13	7 STATES 1 PARENTS	CFP FOR F 13	7 STATES 1 PARENTS
... 7 7 7 ...	
V (1K) FOR F 13	1 STATES	V (1K) FOR F 13	1 STATES	V (1K) FOR F 13	1 STATES
2F 2F 1.224745 -1.224745 1.224745 -1.224745 1.224745 -1.224745 1.224745		2F 2F 1.224745 -1.224745 1.224745 -1.224745 1.224745 -1.224745 1.224745		2F 2F 1.224745 -1.224745 1.224745 -1.224745 1.224745 -1.224745 1.224745	
END		END		END	

