

Supporting Information

Theoretical study of actinide complexes with macropa

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Table S1. Relative Gibbs free energies (kJ/mol) of the eight M(L)⁺ complexes in the gaseous phase and aqueous solution obtained at the TPSSh/LCPP and TPSSh/SCPP levels, respectively. For technical details see text.

Conf ^a	Ac(L) ⁺		La(L) ⁺		Cf(L) ⁺		Lu(L) ⁺	
	LCPP	SCPP	LCPP	SCPP	LCPP	SCPP	LCPP	SCPP
Gas								
δδδ	20.2	25.2			7.2			
δδλ	31.3	32.5			18.8			
δλδ	0.0	0.0	0.0	0.0	4.1	8.3	16.0	17.1
δλλ	18.4	21.0			8.4	13.8		
λδδ	35.2	36.7			24.9	28.5		
λδλ	11.4	14.3	6.4	2.6	0.0	0.0	0.0	0.0
λλδ	36.1	34.7			31.4			
λλλ	25.7	28.0			11.6			
Gas+BSSE								
δδδ	18.4				7.8			
δδλ	31.4				19.4			
δλδ	0.0		0.0	0.0	8.7		21.5	19.5
δλλ	16.6				11.4			
λδδ	34.5				27.1			
λδλ	12.5		4.0	0.8	0.0		0.0	0.0
λλδ	33.6				30.2			
λλλ	23.2				12.2			
Solution								
δδδ	30.8	31.1			2.7			
δδλ	18.8	25.0			28.7			
δλδ	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
δλλ	24.9	15.8			9.4	3.7		
λδδ	49.0	40.1			31.1	17.1		
λδλ	11.5	12.4	30.7	24.5	12.8	4.8	13.7	7.7
λλδ	52.1	38.1			29.8			
λλλ	37.3	36.7			25.4			

^aThe conformers Δ(yyy)(yyy) are abbreviated by the yyy terms.

Table S2. Selected bond distances (Å) of the $\Delta(\delta\lambda\delta)(\delta\lambda\delta)$ and $\Delta(\lambda\delta\lambda)(\lambda\delta\lambda)$ conformers computed with the TPSSh functional.

	Method ^a	M-O ₁	M-O ₂	M-O ₃	M-N ₁	M-N ₂
Ac(L)⁺						
$\delta\lambda\delta$	LCPP	2.441	2.804	2.883	2.742	2.991
	LCPP+BSSE	2.439	2.814	2.905	2.742	3.001
	SCPP	2.431	2.817	2.895	2.736	2.996
$\lambda\delta\lambda$	LCPP	2.444	2.847	2.791	2.762	2.988
	LCPP+BSSE	2.448	2.848	2.785	2.751	2.982
	SCPP	2.430	2.863	2.802	2.756	2.995
La(L)⁺						
$\delta\lambda\delta$	Exp. ^b	2.53/2.55	2.70/2.73	2.79	2.76/2.78	2.90/2.94
	LCPP	2.369	2.747	2.854	2.672	2.957
	LCPP+BSSE	2.364	2.762	2.889	2.672	2.971
	SCPP	2.335	2.752	2.865	2.669	2.966
	SCPP+BSSE	2.334	2.761	2.885	2.668	2.975
$\lambda\delta\lambda$	LCPP	2.387	2.734	2.684	2.676	2.933
	LCPP+BSSE	2.391	2.738	2.678	2.671	2.923
	SCPP	2.355	2.746	2.677	2.671	2.938
	SCPP+BSSE	2.360	2.739	2.675	2.668	2.930
Cf(L)⁺						
$\delta\lambda\delta$	LCPP	2.302	2.683	2.829	2.597	2.933
	LCPP+BSSE	2.298	2.688	2.855	2.594	2.944
	SCPP	2.250	2.667	2.833	2.566	2.930
$\lambda\delta\lambda$	LCPP	2.329	2.649	2.609	2.597	2.900
	LCPP+BSSE	2.330	2.657	2.604	2.593	2.890
	SCPP	2.277	2.633	2.584	2.564	2.889
Lu(L)⁺						
$\delta\lambda\delta$	LCPP	2.182	2.596	2.812	2.518	2.942
	LCPP+BSSE	2.178	2.569	2.836	2.516	2.975
	SCPP	2.158	2.581	2.819	2.498	2.943
	SCPP+BSSE	2.158	2.579	2.843	2.490	2.950
$\lambda\delta\lambda$	Exp. ^b	2.24/2.25	2.45/2.50	2.46/2.49	2.49	2.81/2.91
	LCPP	2.213	2.559	2.524	2.518	2.903
	LCPP+BSSE	2.213	2.566	2.527	2.516	2.896
	SCPP	2.190	2.547	2.508	2.500	2.907
	SCPP+BSSE	2.193	2.549	2.509	2.495	2.904

^aWhen SCF converge errors did not hinder, the optimizations have also been performed taking into account the basis set superposition effect (BSSE).

^bFrom Ref. Angew. Chem. Int. Ed., 2017, 56, 14712-14717. The crystal structures correspond to [La(HL)(H₂O)]·(ClO₄)₂ and [Lu(L)]·ClO₄·DMF.

Table S3. Selected topological properties of the of the $\Delta(\delta\lambda\delta)(\delta\lambda\delta)$ and $\Delta(\lambda\delta\lambda)(\lambda\delta\lambda)$ conformers from QTAIM analysis of the TPPSSh/SCPP wavefunctions.

Property		M-O ₁	M-O ₂	M-O ₃	M-N ₁	M-N ₂
Ac(L)⁺						
$\delta\lambda\delta$	DI	0.375	0.157	0.137	0.223	0.147
	ρ	0.060	0.026	0.024	0.037	0.024
	$\nabla^2\rho$	0.207	0.087	0.072	0.106	0.061
$\lambda\delta\lambda$	DI	0.379	0.144	0.155	0.219	0.146
	ρ	0.060	0.025	0.027	0.036	0.024
	$\nabla^2\rho$	0.209	0.078	0.091	0.102	0.061
La(L)⁺						
$\delta\lambda\delta$	DI	0.423	0.152	0.123	0.229	0.139
	ρ	0.069	0.027	0.022	0.039	0.023
	$\nabla^2\rho$	0.242	0.095	0.072	0.114	0.060
$\lambda\delta\lambda$	DI	0.404	0.155	0.168	0.228	0.143
	ρ	0.066	0.028	0.031	0.039	0.024
	$\nabla^2\rho$	0.235	0.095	0.114	0.115	0.064
Cf(L)⁺						
$\delta\lambda\delta$	DI	0.458	0.166	0.118	0.262	0.136
	ρ	0.077	0.029	0.022	0.045	0.022
	$\nabla^2\rho$	0.330	0.110	0.072	0.147	0.062
$\lambda\delta\lambda$	DI	0.428	0.177	0.186	0.260	0.144
	ρ	0.073	0.032	0.035	0.045	0.024
	$\nabla^2\rho$	0.310	0.122	0.141	0.150	0.069
Lu(L)⁺						
$\delta\lambda\delta$	DI	0.387	0.131	0.076	0.209	0.086
	ρ	0.079	0.027	0.017	0.042	0.017
	$\nabla^2\rho$	0.361	0.112	0.062	0.143	0.052
$\lambda\delta\lambda$	DI	0.353	0.139	0.144	0.205	0.089
	ρ	0.073	0.030	0.032	0.041	0.018
	$\nabla^2\rho$	0.333	0.125	0.140	0.144	0.057

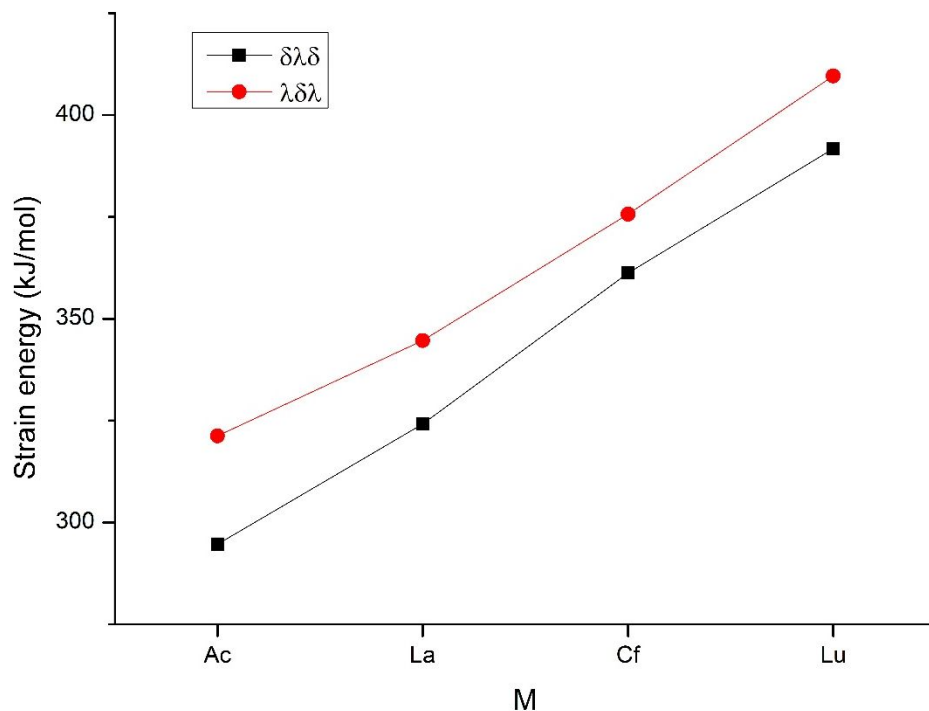


Figure S1. Strain energy of the macropa (L^{2-}) $\Delta(\delta\lambda\delta)(\delta\lambda\delta)$ and $\Delta(\lambda\delta\lambda)(\lambda\delta\lambda)$ conformers in the optimized structures of the respective complexes.

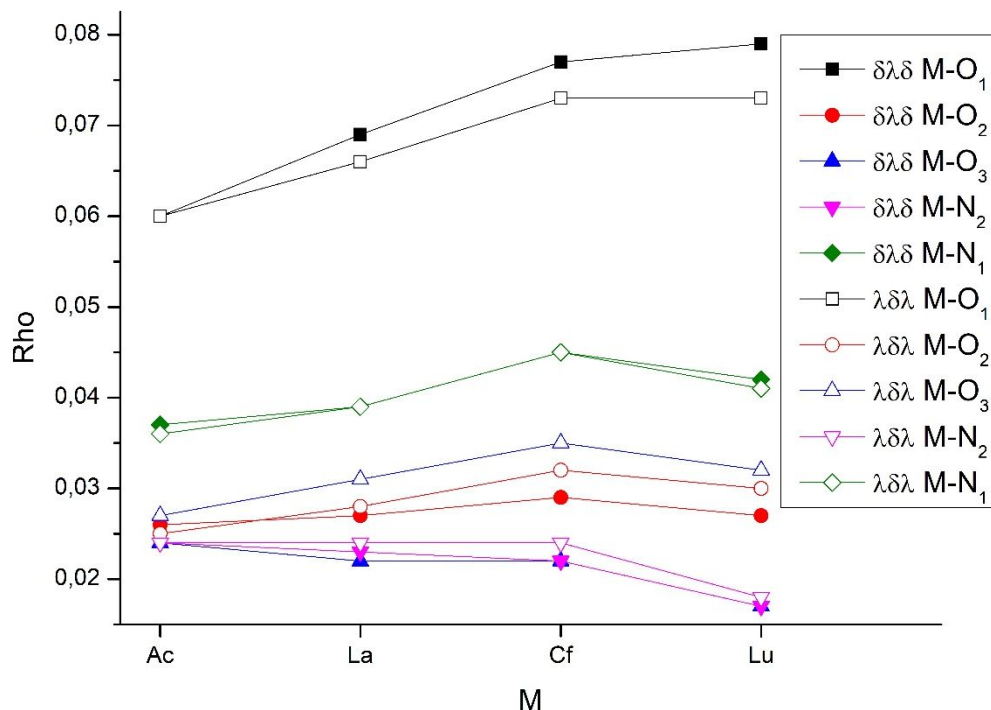


Figure S2. Electron density distribution (ρ , au) at the given bond critical points of the $\Delta(\delta\lambda\delta)(\delta\lambda\delta)$ and $\Delta(\lambda\delta\lambda)(\lambda\delta\lambda)$ complexes.

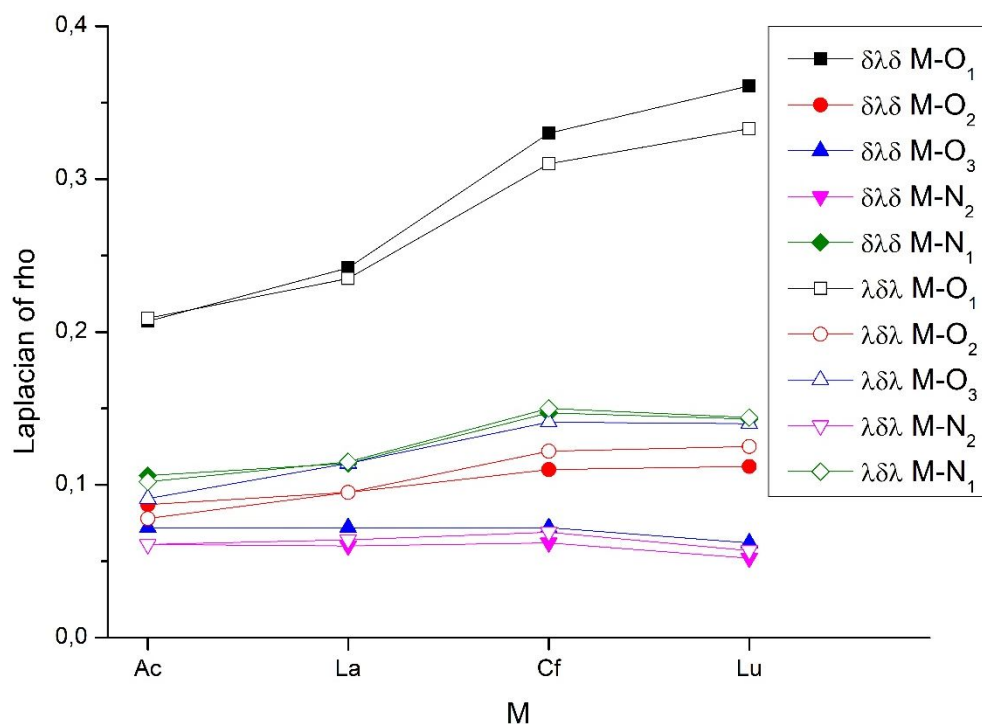


Figure S3. Laplacian of the electron density distribution ($\nabla^2\rho$, au) at the given bond critical points of the $\Delta(\delta\lambda\delta)(\delta\lambda\delta)$ and $\Delta(\lambda\delta\lambda)(\lambda\delta\lambda)$ complexes.

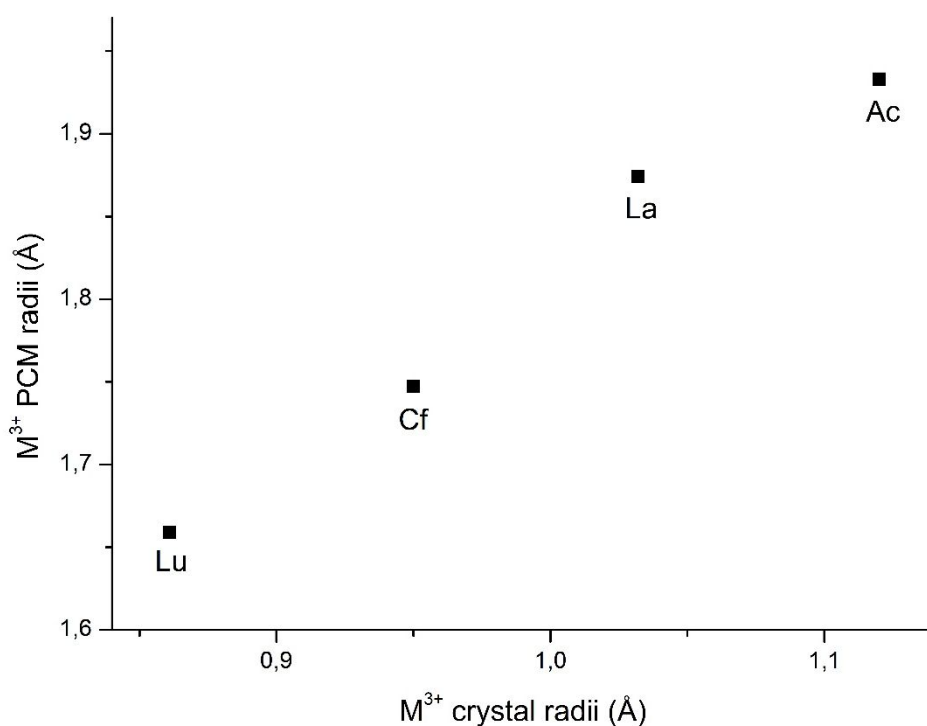


Figure S4. Optimized PCM radii compared with the ionic radii in the crystal (coordination number = 6; no radii for CN=9 are available for Ac^{3+} and Cf^{3+}).

Cartesian coordinates**Ac(L)⁺ Δ(δδδ)(δδδ)**

89	0.000000	0.000000	0.473759
8	2.079871	0.365984	-0.747822
8	-2.079871	-0.365984	-0.747822
8	-1.087955	-2.279796	1.590594
8	2.032521	-0.264731	2.450193
8	1.087955	2.279796	1.590594
8	-2.032521	0.264731	2.450193
7	1.596773	-2.514316	0.634471
7	-1.596773	2.514316	0.634471
7	-0.018965	-1.844085	-1.510177
7	0.018965	1.844085	-1.510177
8	3.211244	0.807920	-2.661566
8	-3.211244	-0.807920	-2.661566
6	0.741540	-3.676214	0.987678
6	-0.259003	-3.346258	2.085227
6	2.712039	-2.394317	1.609272
6	3.154754	-0.960366	1.842770
6	2.387620	0.950836	3.138270
6	2.392922	2.135478	2.184963
6	-2.387620	-0.950836	3.138270
6	-2.392922	-2.135478	2.184963
6	-2.712039	2.394317	1.609272
6	-3.154754	0.960366	1.842770
6	0.259003	3.346258	2.085227
6	-0.741540	3.676214	0.987678
6	2.134140	-2.671739	-0.745935
6	-2.134140	2.671739	-0.745935
6	-1.025889	2.648135	-1.779520
6	1.025889	-2.648135	-1.779520
6	1.067544	1.796105	-2.354465
6	1.093484	2.523809	-3.545374
6	0.000000	3.337030	-3.846952
6	-1.067439	3.416514	-2.946794
6	1.067439	-3.416514	-2.946794
6	0.000000	-3.337030	-3.846952
6	-1.093484	-2.523809	-3.545374
6	-1.067544	-1.796105	-2.354465
1	3.366195	0.833232	3.620451
1	1.630080	1.085051	3.916125
1	3.086355	1.969850	1.356093
1	2.674860	3.055337	2.710148
1	-3.366195	-0.833232	3.620451
1	-1.630080	-1.085051	3.916125
1	-2.674860	-3.055337	2.710148
1	-3.086355	-1.969850	1.356093
1	2.709548	-3.606568	-0.837648
1	2.806503	-1.827498	-0.933334
1	-2.709548	3.606568	-0.837648

1	-2.806503	1.827498	-0.933334
1	1.961574	2.441395	-4.189047
1	-0.016908	3.919659	-4.762813
1	-1.915777	4.063897	-3.144427
1	1.915777	-4.063897	-3.144427
1	0.016908	-3.919659	-4.762813
1	-1.961574	-2.441395	-4.189047
6	2.238208	0.923375	-1.921145
6	-2.238208	-0.923375	-1.921145
1	1.350090	-4.542324	1.292813
1	-0.877442	-4.229316	2.285226
1	0.228363	-3.043841	3.021974
1	-1.350090	4.542324	1.292813
1	-0.173989	3.963066	0.099971
1	0.877442	4.229316	2.285226
1	-0.228363	3.043841	3.021974
1	-3.438637	0.460186	0.910976
1	-3.996589	0.953114	2.545853
1	-2.374628	2.799068	2.567970
1	-3.577958	2.993266	1.288166
1	3.996589	-0.953114	2.545853
1	3.438637	-0.460186	0.910976
1	3.577958	-2.993266	1.288166
1	2.374628	-2.799068	2.567970
1	0.173989	-3.963066	0.099971

Ac(L) ⁺	$\Delta(\delta\delta\lambda)$	$(\delta\delta\lambda)$				
			1	-1.721081	-0.638798	-3.168587
			1	-3.279376	-1.511821	-3.155011
			1	-2.199378	-3.468774	-2.073951
			1	-1.348028	-2.990240	-3.557246
			1	4.023900	1.423518	1.788272
			1	2.284896	1.529027	2.188024
			1	-4.165270	0.569153	-1.942579
			1	-2.499039	1.103566	-2.275179
			1	-2.807588	3.613944	2.894850
			1	-4.860290	3.865730	1.423892
			1	-5.045096	2.436514	-0.621276
			1	4.281886	3.617266	0.659686
			1	3.697988	5.048588	-1.305480
			1	1.831244	4.292735	-2.847789
			6	-0.725987	1.897179	2.484125
			6	0.335853	2.013517	-2.576987
			1	3.763532	0.159090	-0.709130
			1	4.794090	-0.593512	0.518384
			1	4.139272	-2.004934	-1.476836
			1	3.847789	-2.787058	0.086126
			1	-4.240693	-2.072456	-1.047572
			1	-4.074326	-0.812818	0.184279
			1	-3.577419	-2.936554	1.174232
			1	-2.292658	-3.296784	0.000558
89	0.059559	-0.276653				-0.046733
8	0.071570	0.964871				2.036707
8	-0.158982	0.869578				-2.183282
8	2.145532	-2.101536				-0.879720
8	0.743765	-2.072057				1.988965
8	-1.893529	-1.726162				1.310611
8	-0.387049	-2.477024				-1.785973
7	2.772211	-0.175526				1.084031
7	-2.585636	-0.728842				-1.284350
7	1.760055	1.780799				-0.612849
7	-2.053618	1.369572				0.505843
8	-0.572414	2.571851				3.499246
8	-0.016312	2.672468				-3.551308
6	3.779995	-0.592899				0.083100
6	3.540936	-1.953619				-0.558591
6	2.833538	-0.944781				2.351211
6	2.118466	-2.293795				2.337133
6	-0.204290	-3.007767				2.517724
6	-1.532120	-2.272197				2.592541
6	0.504642	-3.601215				-1.787763
6	1.926388	-3.089796				-1.901038
6	-2.335525	-1.347885				-2.607488
6	-1.600081	-2.673775				-2.537506
6	-2.819540	-2.487987				0.519683
6	-3.512559	-1.517646				-0.434441
6	3.003761	1.264476				1.405173
6	-3.146655	0.629937				-1.529426
6	-3.140582	1.482166				-0.280866
6	2.754035	2.160607				0.211902
6	-1.961835	2.117523				1.622739
6	-2.947132	3.037201				1.987862
6	-4.070437	3.165054				1.171295
6	-4.176707	2.369153				0.026357
6	3.479547	3.333809				-0.013942
6	3.151068	4.130187				-1.115690
6	2.126020	3.726332				-1.972014
6	1.456480	2.535105				-1.687791
1	2.338588	-0.333989				3.110031
1	3.877979	-1.104904				2.667486
1	2.174924	-2.709716				3.351106
1	2.558571	-3.020876				1.647239
1	0.095158	-3.319134				3.526758
1	-0.258174	-3.900344				1.878713
1	-1.432018	-1.414235				3.261123
1	-2.325192	-2.932907				2.960905
1	0.292252	-4.253848				-2.642503
1	0.366755	-4.178370				-0.864599
1	2.618634	-3.930942				-1.765734
1	2.101985	-2.635218				-2.883467

Ac(L) ⁺ Δ(δλδ)(δλδ)							
				H	-4.76662400	1.16724700	-0.27204800
				H	-3.75810500	2.44239100	-2.11103700
				H	-3.21606200	3.14219700	-0.57192300
				H	4.76619100	1.16874500	0.27203100
				H	3.66101500	0.18088900	1.24541700
				H	3.75726400	2.44350600	2.11105600
				H	3.21498300	3.14317400	0.57196200
				H	1.88237300	0.60111600	-3.23468000
				H	2.43902300	2.25653100	-3.64279000
				H	3.34961500	2.54234700	-1.38014200
				H	4.17025100	1.25851100	-2.27372200
				H	-2.43980400	2.25564500	3.64282200
				H	-1.88262800	0.60042300	3.23464700
				H	-4.17072000	1.25711500	2.27372600
				H	-3.35050400	2.54125600	1.38019600
				H	-1.04805500	3.89272200	-2.04023600
				H	-2.05600800	3.13632300	-3.30458400
				H	-0.33459800	1.37866300	-3.66235600
				H	0.29195900	3.02789700	-3.97298600
				H	-3.66111900	0.17978400	-1.24546000
				H	2.05495000	3.13687000	3.30461500
				H	1.04675100	3.89296600	2.04027900
				H	-0.29297400	3.02768100	3.97302700
				H	0.33408800	1.37864900	3.66234000
Ac	-0.00005100	0.51782300	0.00011800				
O	-0.39323400	-0.73700700	2.04431400				
O	0.39350700	-0.73659900	-2.04426500				
O	-1.79964600	2.00023400	-1.58158900				
O	-0.94007600	2.13600200	2.20933400				
O	1.79894700	2.00072200	1.58160700				
O	0.93932500	2.13636100	-2.20931800				
N	-2.91946100	0.61129100	0.66517700				
N	2.91920400	0.61221200	-0.66520300				
N	-1.71590800	-1.50579900	-0.66609200				
N	1.71637600	-1.50540200	0.66597100				
O	-0.47289500	-2.68759800	3.19310900				
O	0.47376400	-2.68699900	-3.19334100				
C	-3.70663800	1.00229200	-0.52788000				
C	-3.16590300	2.24861600	-1.20760200				
C	-3.22232100	1.53434300	1.78606100				
C	-2.12634200	1.58777500	2.82949200				
C	0.07849300	2.34028800	3.20075000				
C	1.29189500	2.94645000	2.53942400				
C	-0.07930200	2.34036600	-3.20073300				
C	-1.29289500	2.94613500	-2.53939500				
C	3.22176000	1.53540900	-1.78604900				
C	2.12577000	1.58853000	-2.82948500				
C	3.16512100	2.24956100	1.20761900				
C	3.70626000	1.00343200	0.52786100				
C	-3.26389900	-0.78050100	1.06106400				
C	3.26410700	-0.77944800	-1.06115400				
C	2.84023800	-1.78919700	-0.01734100				
C	-2.83966500	-1.79004600	0.01720400				
C	1.28020600	-2.35847600	1.61451700				
C	1.93508000	-3.55742600	1.89765500				
C	3.09322900	-3.86335600	1.18163100				
C	3.56201900	-2.96303900	0.22080600				
C	-3.56102100	-2.96413400	-0.22101600				
C	-3.09190900	-3.86421600	-1.18190500				
C	-1.93387400	-3.55781500	-1.89791700				
C	-1.27943200	-2.35864900	-1.61469500				
H	-4.34505800	-0.87341200	1.25256900				
H	-2.72613500	-1.00156800	1.98888900				
H	4.34529200	-0.87198400	-1.25268900				
H	2.72639600	-1.00064800	-1.98897800				
H	1.52856400	-4.20485000	2.66595000				
H	3.63478500	-4.78400900	1.37555800				
H	4.47055700	-3.16605000	-0.33697600				
H	-4.46948600	-3.16750900	0.33675200				
H	-3.63313200	-4.78505200	-1.37589000				
H	-1.52712600	-4.20503600	-2.66626100				
C	0.03272100	-1.92909600	2.36928600				
C	-0.03209800	-1.92876400	-2.36942400				

Ac(L)⁺ Δ(δλλ)(δλλ)

				1	1.642728	-4.408684	1.269820
				1	-0.605714	-4.249264	2.311238
89	0.000000	0.000000	0.420114	1	0.521794	-3.128762	3.089971
8	2.149998	0.297523	-0.702350	1	-1.642728	4.408684	1.269820
8	-2.149998	-0.297523	-0.702350	1	-0.322675	4.006358	0.164070
8	-0.865747	-2.248374	1.824835	1	0.605714	4.249264	2.311238
8	1.986319	-0.235377	2.446041	1	-0.521794	3.128762	3.089971
8	0.865747	2.248374	1.824835	1	-1.576275	-1.998183	3.764655
8	-1.986319	0.235377	2.446041	1	-2.571540	-3.044996	2.707996
7	1.658298	-2.431714	0.440206	1	-3.182583	-1.051176	1.317784
7	-1.658298	2.431714	0.440206	1	-3.655075	-0.864613	3.040290
7	-0.214098	-1.893904	-1.544262	1	0.322675	-4.006358	0.164070
7	0.214098	1.893904	-1.544262	1	2.571540	3.044996	2.707996
8	3.461958	0.810657	-2.476175	1	1.576275	1.998183	3.764655
8	-3.461958	-0.810657	-2.476175	1	3.655075	0.864613	3.040290
6	0.937264	-3.613551	0.977734	1	3.182583	1.051176	1.317784
6	0.000000	-3.347148	2.151014	1	3.532193	-3.031951	1.288929
6	2.920826	-2.122497	1.157000	1	3.474389	-1.427468	0.520504
6	2.727075	-1.472748	2.522266	1	3.711161	-1.279689	2.965265
6	2.811797	0.945699	2.343624	1	2.176094	-2.108432	3.216824
6	1.964224	2.131254	2.746298	1	-2.176094	2.108432	3.216824
6	-2.811797	-0.945699	2.343624	1	-3.711161	1.279689	2.965265
6	-1.964224	-2.131254	2.746298	1	-3.474389	1.427468	0.520504
6	-2.920826	2.122497	1.157000	1	-3.532193	3.031951	1.288929
6	-2.727075	1.472748	2.522266				
6	0.000000	3.347148	2.151014				
6	-0.937264	3.613551	0.977734				
6	2.005799	-2.698693	-0.986383				
6	-2.005799	2.698693	-0.986383				
6	-0.777722	2.744544	-1.867965				
6	0.777722	-2.744544	-1.867965				
6	1.340845	1.872591	-2.283710				
6	1.509521	2.680714	-3.409103				
6	0.477862	3.552795	-3.758718				
6	-0.676756	3.597464	-2.971678				
6	0.676756	-3.597464	-2.971678				
6	-0.477862	-3.552795	-3.758718				
6	-1.509521	-2.680714	-3.409103				
6	-1.340845	-1.872591	-2.283710				
1	2.574262	-3.636523	-1.085002				
1	2.643686	-1.872402	-1.316140				
1	-2.574262	3.636523	-1.085002				
1	-2.643686	1.872402	-1.316140				
1	2.436286	2.609898	-3.966601				
1	0.573276	4.201617	-4.623857				
1	-1.486648	4.280337	-3.207671				
1	1.486648	-4.280337	-3.207671				
1	-0.573276	-4.201617	-4.623857				
1	-2.436286	-2.609898	-3.966601				
6	2.433237	0.924382	-1.814305				
6	-2.433237	-0.924382	-1.814305				

Ac(L) ⁺ Δ(λδδ)(λδδ)			
			1 -2.064236 -2.968107 -0.032701
			1 -2.498140 -3.812814 1.473323
			1 -0.253196 -4.047608 2.184244
			1 -0.380824 -4.727903 0.561276
			1 -1.441535 4.269375 -0.768652
			1 -2.109421 2.618964 -0.843977
			1 1.441535 -4.269375 -0.768652
			1 2.109421 -2.618964 -0.843977
			1 -2.423147 -1.504991 -4.217943
			1 -1.076248 -3.584288 -4.759776
			1 0.578320 -4.412147 -3.080032
			1 -0.578320 4.412147 -3.080032
			1 1.076248 3.584288 -4.759776
			1 2.423147 1.504991 -4.217943
			6 -2.273019 -0.055174 -1.884753
			6 2.273019 0.055174 -1.884753
			1 3.649649 -2.178460 2.440788
			1 3.211738 -1.590550 0.801340
			1 2.489883 -4.000233 1.366499
			1 1.493033 -3.307972 2.656444
			1 -3.649649 2.178460 2.440788
			1 -3.211738 1.590550 0.801340
			1 -1.493033 3.307972 2.656444
			1 -2.489883 4.000233 1.366499
89	0.000000	0.000000	0.639363
8	-2.072758	0.282971	-0.637612
8	2.072758	-0.282971	-0.637612
8	1.734698	1.896834	1.720615
8	-2.054741	0.844619	2.371590
8	-1.734698	-1.896834	1.720615
8	2.054741	-0.844619	2.371590
7	-0.751829	2.909596	0.729830
7	0.751829	-2.909596	0.729830
7	0.531783	1.688307	-1.441100
7	-0.531783	-1.688307	-1.441100
8	-3.031706	0.492985	-2.681071
8	3.031706	-0.492985	-2.681071
6	0.386602	3.787349	1.131383
6	1.763181	3.146314	1.002570
6	-1.897898	3.118615	1.659256
6	-2.821961	1.919720	1.769140
6	-2.855069	-0.206260	2.947765
6	-3.046839	-1.359712	1.983171
6	2.855069	0.206260	2.947765
6	3.046839	1.359712	1.983171
6	1.897898	-3.118615	1.659256
6	2.821961	-1.919720	1.769140
6	-1.763181	-3.146314	1.002570
6	-0.386602	-3.787349	1.131383
6	-1.199266	3.200186	-0.660124
6	1.199266	-3.200186	-0.660124
6	0.181467	-2.797681	-1.703563
6	-0.181467	2.797681	-1.703563
6	-1.457149	-1.260964	-2.323290
6	-1.675969	-1.904112	-3.541758
6	-0.929015	-3.048695	-3.827081
6	0.000000	-3.513448	-2.891521
6	0.000000	3.513448	-2.891521
6	0.929015	3.048695	-3.827081
6	1.675969	1.904112	-3.541758
6	1.457149	1.260964	-2.323290
1	0.253196	4.047608	2.184244
1	0.380824	4.727903	0.561276
1	2.498140	3.812814	1.473323
1	2.064236	2.968107	-0.032701
1	-3.825731	0.193755	3.261544
1	-2.313471	-0.551330	3.833208
1	-3.506378	-1.032114	1.043692
1	-3.669783	-2.132802	2.452600
1	3.825731	-0.193755	3.261544
1	2.313471	0.551330	3.833208
1	3.669783	2.132802	2.452600
1	3.506378	1.032114	1.043692

Ac(L)⁺ Δ(λδλ)(λδλ)

				1	2.147926	-2.622988	3.601353
				1	1.332979	-1.092837	4.022578
89	0.000000	0.000000	0.340675	1	3.661848	-0.686850	3.253223
8	-1.061301	1.800758	-0.899341	1	3.321659	-1.547704	1.721138
8	1.061301	-1.800758	-0.899341	1	0.238913	-3.702395	0.372570
8	2.341979	0.276238	1.964319	1	-1.083343	-4.557648	1.213034
8	-0.754280	1.945948	2.210200	1	-0.758061	-2.985424	3.189855
8	-2.341979	-0.276238	1.964319	1	0.674579	-3.945953	2.762382
8	0.754280	-1.945948	2.210200	1	-3.682086	-0.706239	0.429639
7	1.512414	2.581054	0.490468	1	-4.223702	-1.156388	2.065321
7	-1.512414	-2.581054	0.490468	1	-2.588765	-2.890430	2.273192
7	1.960582	0.611533	-1.497846	1	-3.540075	-3.184290	0.818414
7	-1.960582	-0.611533	-1.497846	1	2.359895	3.880491	-0.985882
8	-2.276336	2.762538	-2.553557	1	0.773475	3.161307	-1.367191
8	2.276336	-2.762538	-2.553557	1	-2.359895	-3.880491	-0.985882
6	2.780628	2.523198	1.261730	1	-0.773475	-3.161307	-1.367191
6	3.359549	1.122620	1.388900	1	-3.724694	1.091711	-3.802295
6	0.585961	3.582685	1.078986	1	-4.588466	-1.250397	-4.264506
6	0.000000	3.153976	2.413895	1	-3.704241	-3.141017	-2.884997
6	-1.757954	1.680424	3.198624	1	3.704241	3.141017	-2.884997
6	-2.884252	0.933858	2.518137	1	4.588466	1.250397	-4.264506
6	1.757954	-1.680424	3.198624	1	3.724694	-1.091711	-3.802295
6	2.884252	-0.933858	2.518137	6	-1.902860	1.794006	-1.897109
6	-0.585961	-3.582685	1.078986	6	1.902860	-1.794006	-1.897109
6	0.000000	-3.153976	2.413895				
6	-3.359549	-1.122620	1.388900				
6	-2.780628	-2.523198	1.261730				
6	1.756006	2.961592	-0.925624				
6	-1.756006	-2.961592	-0.925624				
6	-2.404652	-1.861843	-1.733402				
6	2.404652	1.861843	-1.733402				
6	-2.442974	0.411554	-2.232211				
6	-3.385557	0.225976	-3.245290				
6	-3.850750	-1.065937	-3.489667				
6	-3.359531	-2.125162	-2.720164				
6	3.359531	2.125162	-2.720164				
6	3.850750	1.065937	-3.489667				
6	3.385557	-0.225976	-3.245290				
6	2.442974	-0.411554	-2.232211				
1	2.588765	2.890430	2.273192				
1	3.540075	3.184290	0.818414				
1	4.223702	1.156388	2.065321				
1	3.682086	0.706239	0.429639				
1	-0.238913	3.702395	0.372570				
1	1.083343	4.557648	1.213034				
1	-0.674579	3.945953	2.762382				
1	0.758061	2.985424	3.189855				
1	-2.147926	2.622988	3.601353				
1	-1.332979	1.092837	4.022578				
1	-3.321659	1.547704	1.721138				
1	-3.661848	0.686850	3.253223				

Ac(L)+ $\Delta(\lambda\lambda\delta)(\lambda\lambda\delta)$

				1	1.456331	4.236848	-2.465485
				1	3.542424	4.785107	-1.135277
				1	4.417954	3.093422	0.481383
				1	-4.108534	3.493524	-0.481463
				1	-3.078418	5.095633	1.135336
				1	-1.053013	4.354178	2.465708
				6	0.024836	1.877949	-2.310337
				6	0.151176	1.871484	2.310395
				1	2.413341	-2.556926	3.413833
				1	1.937950	-0.850054	3.146635
				1	4.124564	-1.650853	2.001928
				1	3.106579	-2.741250	1.041205
				1	-2.642577	-2.320003	-3.413589
				1	-2.008958	-0.665314	-3.146247
				1	-3.349934	-2.438421	-1.040762
				1	-4.261097	-1.257400	-2.001623
				1	0.249442	-1.520633	-3.576606
				1	-0.494114	-3.122055	-3.857984
				1	1.843400	-3.472006	-3.140455
				1	0.721491	-4.049055	-1.882587
				1	-0.391237	-1.490107	3.576780
				1	0.199531	-3.154011	3.858056
				1	-1.097121	-3.963406	1.882647
				1	-2.160378	-3.284268	3.140477
89	-0.028101	-0.598677	-0.000142				
8	-0.295768	0.625069	-2.108684				
8	0.352625	0.594017	2.108799				
8	-1.912462	-2.173329	1.392991				
8	-1.049073	-2.171899	-2.090640				
8	1.700241	-2.342721	-1.393041				
8	0.840834	-2.259671	2.090808				
7	-2.923843	-0.454575	-0.532777				
7	2.868546	-0.726290	0.532879				
7	-1.561639	1.587187	0.620882				
7	1.703596	1.434190	-0.620954				
8	-0.560763	2.675812	-3.038929				
8	0.808959	2.610804	3.039150				
6	-3.696271	-0.709964	0.722169				
6	-2.803263	-1.143220	1.881709				
6	-3.278112	-1.475563	-1.553165				
6	-2.254874	-1.617305	-2.664503				
6	-0.062941	-2.456983	-3.097147				
6	1.088366	-3.163488	-2.407537				
6	-0.167643	-2.451506	3.097285				
6	-1.379821	-3.047495	2.407604				
6	3.125440	-1.775840	1.553491				
6	2.093362	-1.820868	2.664780				
6	2.683776	-1.400712	-1.881605				
6	3.613525	-1.053294	-0.722032				
6	-3.181450	0.916872	-1.044798				
6	3.253529	0.615030	1.044697				
6	2.819179	1.698518	0.080985				
6	-2.647498	1.954934	-0.081092				
6	1.248089	2.323947	-1.524725				
6	1.872392	3.553193	-1.734515				
6	3.022348	3.842452	-0.995840				
6	3.514329	2.900325	-0.087617				
6	-3.226996	3.216583	0.087551				
6	-2.648965	4.108391	0.995884				
6	-1.531241	3.712580	1.734640				
6	-1.024854	2.430269	1.524795				
1	-4.453040	-1.479590	0.535938				
1	-4.227557	0.197412	1.027991				
1	-3.417916	-1.547581	2.695281				
1	-2.214417	-0.301763	2.266856				
1	2.176549	-0.507657	-2.266669				
1	3.257776	-1.860855	-2.695236				
1	4.294383	-1.890794	-0.535699				
1	4.228010	-0.200048	-1.027862				
1	-4.256833	1.079409	-1.218806				
1	-2.656468	1.030856	-1.999176				
1	4.339405	0.676144	1.218728				
1	2.741588	0.777807	1.999081				

Ac(L)⁺ Δ(λλλ)(λλλ)

				1	-2.828016	-2.364405	-3.840056
				1	-1.341629	-4.368699	-4.304764
89	0.000000	0.000000	0.462614	1	0.652896	-4.739306	-2.841635
8	-2.089078	0.131704	-0.797914	1	-0.652896	4.739306	-2.841635
8	2.089078	-0.131704	-0.797914	1	1.341629	4.368699	-4.304764
8	1.339187	2.136666	1.612926	1	2.828016	2.364405	-3.840056
8	-2.058918	0.347244	2.394777	6	-2.491961	-0.533232	-1.848392
8	-1.339187	-2.136666	1.612926	6	2.491961	0.533232	-1.848392
8	2.058918	-0.347244	2.394777	1	-3.404712	-0.451251	1.019861
7	1.281543	-2.668927	0.617273	1	-3.975531	-0.405948	2.722884
7	0.520779	1.911260	-1.432987	1	-3.325538	-2.701521	1.931342
7	-0.520779	-1.911260	-1.432987	1	-2.421912	-2.167037	3.379026
7	-1.281543	2.668927	0.617273	1	3.404712	0.451251	1.019861
8	-3.484508	-0.292539	-2.531026	1	3.975531	0.405948	2.722884
8	3.484508	0.292539	-2.531026	1	2.421912	2.167037	3.379026
6	-0.494828	3.678824	1.368712	1	3.325538	2.701521	1.931342
6	1.015253	3.500644	1.275741	1	1.807655	-2.151372	3.277758
6	-2.607968	2.474853	1.264859	1	3.500350	-1.690216	3.062996
6	-2.517019	1.702810	2.577530	1	3.102296	-3.442164	1.455845
6	-3.113649	-0.582960	2.067125	1	3.226142	-1.911751	0.560984
6	-2.589874	-1.982915	2.311159	1	-3.500350	1.690216	3.062996
6	3.113649	0.582960	2.067125	1	-1.807655	2.151372	3.277758
6	2.589874	1.982915	2.311159	1	-3.102296	3.442164	1.455845
6	2.607968	-2.474853	1.264859	1	-3.226142	1.911751	0.560984
6	2.517019	-1.702810	2.577530				
6	-1.015253	-3.500644	1.275741				
6	0.494828	-3.678824	1.368712				
6	-1.506821	3.089125	-0.791796				
6	1.506821	-3.089125	-0.791796				
6	0.273426	-2.974936	-1.659089				
6	-0.273426	2.974936	-1.659089				
6	-1.612340	-1.723089	-2.201793				
6	-1.941216	-2.578624	-3.254860				
6	-1.116562	-3.677156	-3.498727				
6	0.000000	-3.886707	-2.684134				
6	0.000000	3.886707	-2.684134				
6	1.116562	3.677156	-3.498727				
6	1.941216	2.578624	-3.254860				
6	1.612340	1.723089	-2.201793				
1	-0.764757	3.600851	2.424433				
1	-0.754334	4.698976	1.043688				
1	1.484563	4.177942	1.999076				
1	1.411992	3.722950	0.280907				
1	-1.411992	-3.722950	0.280907				
1	-1.484563	-4.177942	1.999076				
1	0.764757	-3.600851	2.424433				
1	0.754334	-4.698976	1.043688				
1	-1.902937	4.115689	-0.834341				
1	-2.259875	2.408018	-1.202432				
1	1.902937	-4.115689	-0.834341				
1	2.259875	-2.408018	-1.202432				

cf(L)* $\Delta(\delta\lambda\delta)(\delta\lambda\delta)$

				1	4.684787	-0.368839	0.834339
				1	3.612487	-2.181813	2.152882
				1	3.367584	-0.607642	2.934636
				1	-4.684787	0.368839	0.834339
				1	-3.435661	1.251603	-0.062914
				1	-3.612487	2.181813	2.152882
				1	-3.367584	0.607642	2.934636
				1	-1.775166	-3.228662	0.774183
				1	-2.436679	-3.464334	2.425735
				1	-3.506342	-1.285177	2.375445
				1	-4.120940	-2.297884	1.069120
				1	2.436679	3.464334	2.425735
				1	1.775166	3.228662	0.774183
				1	4.120940	2.297884	1.069120
				1	3.506342	1.285177	2.375445
				1	0.956276	-1.380945	3.916845
				1	1.970993	-2.785193	3.494786
				1	0.276383	-3.571756	1.875185
				1	-0.387601	-3.473934	3.535159
				1	3.435661	-1.251603	-0.062914
				1	-1.970993	2.785193	3.494786
				1	-0.956276	1.380945	3.916845
				1	0.387601	3.473934	3.535159
				1	-0.276383	3.571756	1.875185
98	0.000000	0.000000	0.463144				
8	0.345382	2.005564	-0.496484				
8	-0.345382	-2.005564	-0.496484				
8	1.703549	-1.390240	1.972417				
8	0.999989	1.975892	2.229325				
8	-1.703549	1.390240	1.972417				
8	-0.999989	-1.975892	2.229325				
7	2.848743	0.686178	0.468392				
7	-2.848743	-0.686178	0.468392				
7	1.513403	-0.553770	-1.533438				
7	-1.513403	0.553770	-1.533438				
8	0.717939	3.144755	-2.414641				
8	-0.717939	-3.144755	-2.414641				
6	3.599867	-0.552750	0.759936				
6	3.126570	-1.203480	2.045004				
6	3.235259	1.749465	1.424917				
6	2.109216	2.722489	1.684865				
6	0.000000	2.889302	2.688878				
6	-1.203451	2.096660	3.122523				
6	0.000000	-2.889302	2.688878				
6	1.203451	-2.096660	3.122523				
6	-3.235259	-1.749465	1.424917				
6	-2.109216	-2.722489	1.684865				
6	-3.126570	1.203480	2.045004				
6	-3.599867	0.552750	0.759936				
6	3.125480	1.141174	-0.914541				
6	-3.125480	-1.141174	-0.914541				
6	-2.589117	-0.153694	-1.922134				
6	2.589117	0.153694	-1.922134				
6	-1.028361	1.517270	-2.341925				
6	-1.551153	1.771935	-3.607029				
6	-2.641755	1.010680	-4.032306				
6	-3.181270	0.051341	-3.172811				
6	3.181270	-0.051341	-3.172811				
6	2.641755	-1.010680	-4.032306				
6	1.551153	-1.771935	-3.607029				
6	1.028361	-1.517270	-2.341925				
1	4.207026	1.281203	-1.074791				
1	2.630834	2.107177	-1.062182				
1	-4.207026	-1.281203	-1.074791				
1	-2.630834	-2.107177	-1.062182				
1	-1.106269	2.555118	-4.209988				
1	-3.084052	1.177153	-5.009539				
1	-4.051941	-0.528790	-3.460638				
1	4.051941	0.528790	-3.460638				
1	3.084052	-1.177153	-5.009539				
1	1.106269	-2.555118	-4.209988				
6	0.108231	2.314352	-1.747366				
6	-0.108231	-2.314352	-1.747366				

cf(L)* $\Delta(\delta\lambda\lambda)(\delta\lambda\lambda)$

				1	-0.864133	4.689769	0.228412
				1	-1.795747	3.675531	2.360323
				1	-2.829747	3.421917	0.949357
				1	-0.864164	-4.689758	-0.228426
				1	0.206061	-3.633733	-1.160402
				1	-1.795786	-3.675503	-2.360328
				1	-2.829781	-3.421904	-0.949355
				1	-3.748716	1.403364	2.007383
				1	-2.728727	1.859075	3.403969
				1	-1.516269	-0.291012	3.272387
				1	-3.289689	-0.571503	3.388708
				1	0.206095	3.633748	1.160387
				1	-2.728762	-1.859051	-3.403958
				1	-3.748749	-1.403319	-2.007377
				1	-3.289688	0.571537	-3.388709
				1	-1.516273	0.291017	-3.272384
				1	-1.501079	4.089742	-1.941439
				1	-0.805297	2.627855	-2.674503
				1	-3.272829	2.497832	-2.490094
				1	-3.178733	2.589768	-0.730988
				1	-3.178755	-2.589730	0.730981
				1	-3.272850	-2.497800	2.490087
				1	-0.805319	-2.627853	2.674496
				1	-1.501118	-4.089728	1.941426
98	-0.445934	-0.000002	0.000004				
8	0.418231	0.423336	-2.052956				
8	0.418228	-0.423344	2.052945				
8	-1.750166	1.758961	1.569975				
8	-2.454991	0.861776	-1.502414				
8	-1.750205	-1.758941	-1.569962				
8	-2.454996	-0.861749	1.502413				
7	-0.389113	2.791307	-0.645139				
7	-0.389135	-2.791302	0.645131				
7	1.541323	1.451922	0.643053				
7	1.541316	-1.451936	-0.643058				
8	2.289308	0.788366	-3.270264				
8	2.289296	-0.788382	3.270263				
6	-0.685218	3.644557	0.529622				
6	-1.852324	3.175310	1.384048				
6	-1.305284	3.015630	-1.783676				
6	-2.634437	2.286268	-1.624075				
6	-2.479687	0.170003	-2.767777				
6	-2.760263	-1.281771	-2.470542				
6	-2.479680	-0.169980	2.767779				
6	-2.760233	1.281800	2.470551				
6	-1.305311	-3.015618	1.783667				
6	-2.634456	-2.286239	1.624069				
6	-1.852360	-3.175292	-1.384048				
6	-0.685249	-3.644545	-0.529632				
6	1.007696	3.077790	-1.066205				
6	1.007671	-3.077802	1.066196				
6	1.973535	-2.526222	0.042023				
6	1.973552	2.526204	-0.042028				
6	2.293737	-0.954481	-1.643801				
6	3.551804	-1.462460	-1.959581				
6	4.026977	-2.547497	-1.220135				
6	3.221453	-3.100498	-0.221693				
6	3.221473	3.100472	0.221689				
6	4.026991	2.547470	1.220136				
6	3.551809	1.462438	1.959581				
6	2.293741	0.954465	1.643798				
1	1.175658	4.159538	-1.187452				
1	1.182648	2.598370	-2.034054				
1	1.175620	-4.159553	1.187438				
1	1.182628	-2.598389	2.034048				
1	4.110785	-1.010606	-2.770869				
1	5.000633	-2.977001	-1.434450				
1	3.547665	-3.969170	0.341022				
1	3.547691	3.969140	-0.341027				
1	5.000649	2.976969	1.434452				
1	4.110784	1.010582	2.770872				
6	1.654406	0.179376	-2.413450				
6	1.654404	-0.179389	2.413445				

cf(L)* $\Delta(\lambda\delta\delta)(\lambda\delta\delta)$

				1	0.063216	-2.401395	-2.346224
				1	-1.352501	-3.392744	-2.777118
				1	-1.607459	-4.308232	-0.635936
				1	0.131053	-4.351681	-0.897123
				1	0.985688	4.196090	-1.259287
				1	0.863657	2.612660	-2.063788
				1	0.985990	-4.196025	1.259215
				1	0.863883	-2.612621	2.063755
				1	4.205851	-1.010107	-2.453646
				1	4.987346	-2.994361	-1.078251
				1	3.401183	-4.013119	0.561305
				1	3.400838	4.013371	-0.561360
				1	4.987102	2.994740	1.078181
				1	4.205773	1.010418	2.453576
				6	1.704154	0.159828	-2.281566
				6	1.704190	-0.159716	2.281520
				1	-2.760603	-2.343585	3.071856
				1	-1.089970	-1.690184	2.967440
				1	-1.336434	-4.087363	2.112892
				1	-2.508939	-3.471931	0.934256
				1	-2.760823	2.343316	-3.071861
				1	-1.090151	1.690018	-2.967415
				1	-2.509196	3.471865	-0.934374
				1	-1.336696	4.087235	-2.113044
98	-0.551062	-0.000049	0.000008				
8	0.433316	0.358622	-2.019473				
8	0.433367	-0.358631	2.019439				
8	-1.749531	1.707982	1.626929				
8	-2.432836	0.985003	-1.530762				
8	-1.749598	-1.708080	-1.626845				
8	-2.432717	-0.985135	1.530860				
7	-0.541201	2.888514	-0.516665				
7	-0.540956	-2.888502	0.516613				
7	1.485273	1.470562	0.526888				
7	1.485414	-1.470458	-0.526926				
8	2.381406	0.782283	-3.093426				
8	2.381503	-0.782108	3.093376				
6	-0.719906	3.678218	0.738116				
6	-0.884915	2.803223	1.978366				
6	-1.606774	3.216992	-1.494427				
6	-1.949604	2.049134	-2.395258				
6	-3.237927	0.007238	-2.215908				
6	-2.369057	-1.099763	-2.770608				
6	-3.237738	-0.007396	2.216132				
6	-2.368826	1.099613	2.770751				
6	-1.606531	-3.217079	1.494342				
6	-1.949410	-2.049305	2.395265				
6	-0.884847	-2.803184	-1.978390				
6	-0.719599	-3.678200	-0.738187				
6	0.803508	3.121844	-1.096712				
6	0.803764	-3.121784	1.096666				
6	1.857133	-2.558812	0.169499				
6	1.856907	2.558946	-0.169538				
6	2.308912	-0.961111	-1.463547				
6	3.586062	-1.467879	-1.691214				
6	4.000805	-2.565463	-0.932688				
6	3.120058	-3.133786	-0.008954				
6	3.119790	3.134017	0.008904				
6	4.000593	2.565765	0.932627				
6	3.585943	1.468146	1.691152				
6	2.308831	0.961278	1.463495				
1	-1.607902	4.308064	0.635904				
1	0.130620	4.351881	0.896972				
1	-1.352598	3.392748	2.777105				
1	0.063236	2.401597	2.346149				
1	-3.819362	0.490674	-3.008602				
1	-3.924344	-0.400125	-1.468707				
1	-1.599952	-0.710601	-3.448700				
1	-2.981911	-1.842703	-3.298174				
1	-3.819062	-0.490865	3.008887				
1	-3.924258	0.399969	1.469027				
1	-2.981645	1.842517	3.298412				
1	-1.599626	0.710459	3.448739				

cf(L)* $\Delta(\lambda\delta\lambda)(\lambda\delta\lambda)$

98 0.459880 0.000000 0.000000
 8 -0.417952 -0.308377 -2.077705
 8 -0.417950 0.308375 2.077706
 8 1.788606 -1.781125 1.412459
 8 2.449755 -0.837002 -1.420797
 8 1.788607 1.781118 -1.412463
 8 2.449757 0.836997 1.420799
 7 0.423072 -2.784423 -0.770128
 7 0.423080 2.784420 0.770128
 7 -1.528453 -1.507754 0.588439
 7 -1.528448 1.507756 -0.588438
 8 -2.336238 -0.712535 -3.211425
 8 -2.336237 0.712547 3.211419
 6 0.867098 -3.689424 0.325694
 6 1.022175 -2.974536 1.661574
 6 1.314785 -2.892524 -1.945808
 6 2.661329 -2.239760 -1.681204
 6 3.255521 0.087370 -2.167622
 6 2.363077 1.225877 -2.607462
 6 3.255523 -0.087379 2.167619
 6 2.363079 -1.225885 2.607458
 6 1.314793 2.892521 1.945809
 6 2.661336 2.239754 1.681209
 6 1.022182 2.974533 -1.661575
 6 0.867109 3.689420 -0.325694
 6 -0.974555 -3.069941 -1.169656
 6 -0.974545 3.069942 1.169657
 6 -1.934471 2.582461 0.110563
 6 -1.934478 -2.582458 -0.110561
 6 -2.295365 1.038213 -1.593092
 6 -3.542369 1.577780 -1.898918
 6 -3.985522 2.672346 -1.152872
 6 -3.165285 3.194597 -0.150247
 6 -3.165293 -3.194592 0.150251
 6 -3.985528 -2.672339 1.152876
 6 -3.542373 -1.577771 1.898920
 6 -2.295368 -1.038208 1.593093
 1 1.834217 -4.124741 0.055664
 1 0.166269 -4.525339 0.447446
 1 1.572073 -3.618559 2.359925
 1 0.063420 -2.701373 2.111729
 1 0.829125 -2.361855 -2.767558
 1 1.473715 -3.942397 -2.243356
 1 3.301115 -2.356374 -2.562183
 1 3.177430 -2.673904 -0.818264
 1 3.679843 -0.405025 -3.049131
 1 4.072592 0.451692 -1.534038
 1 1.564768 0.863378 -3.264650
 1 2.956601 1.992811 -3.122283

1 3.679849 0.405012 3.049128
 1 4.072592 -0.451701 1.534031
 1 2.956602 -1.992821 3.122277
 1 1.564771 -0.863387 3.264648
 1 0.829131 2.361853 2.767559
 1 1.473724 3.942394 2.243356
 1 3.177442 2.673898 0.818272
 1 3.301118 2.356364 2.562191
 1 0.063426 2.701377 -2.111732
 1 1.572084 3.618555 -2.359925
 1 1.834229 4.124733 -0.055665
 1 0.166282 4.525338 -0.447444
 1 -1.129847 -4.145519 -1.347804
 1 -1.179270 -2.540135 -2.106474
 1 -1.129835 4.145520 1.347804
 1 -1.179262 2.540137 2.106476
 1 -4.116594 1.145051 -2.710020
 1 -4.947083 3.130097 -1.363424
 1 -3.469191 4.065094 0.422050
 1 -3.469202 -4.065089 -0.422044
 1 -4.947090 -3.130087 1.363429
 1 -4.116597 -1.145040 2.710021
 6 -1.672950 -0.091750 -2.384507
 6 -1.672950 0.091756 2.384505