Supporting Information

For

On the Origins of Kinetic Resolution of Cyclohexane-1,2-diols Through Stereoselective Acylation by Chiral Tetrapeptides

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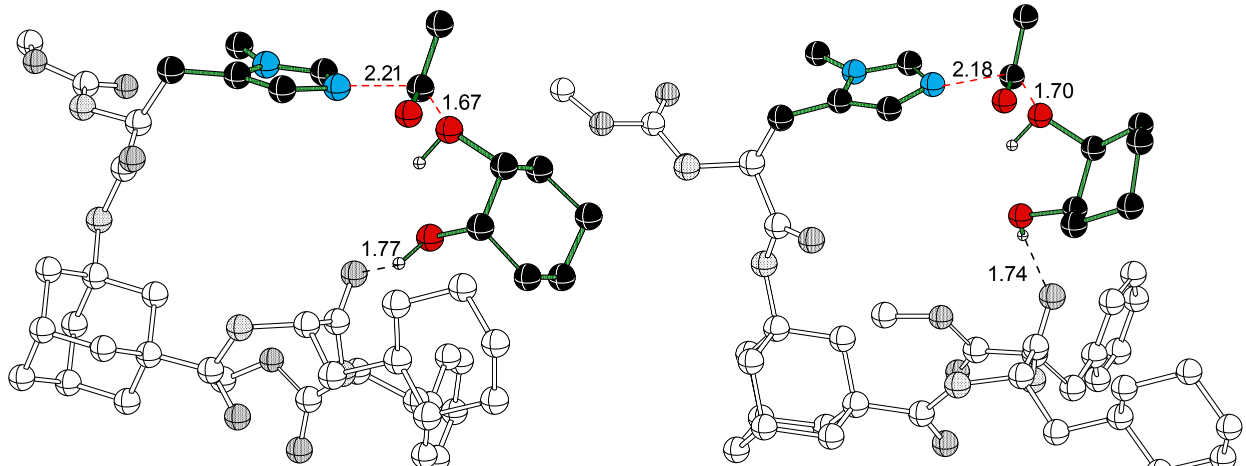
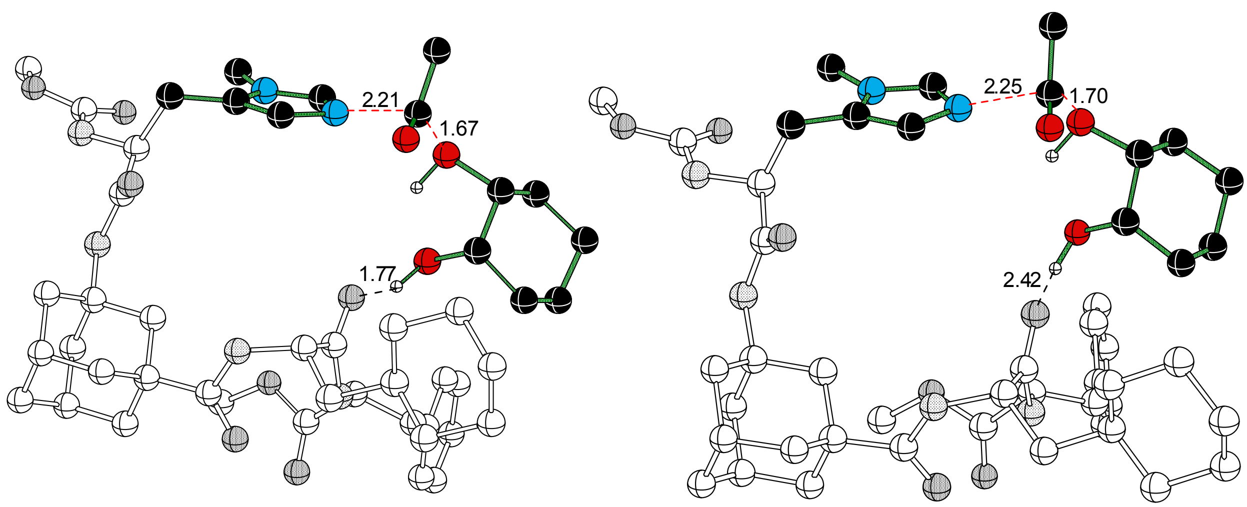


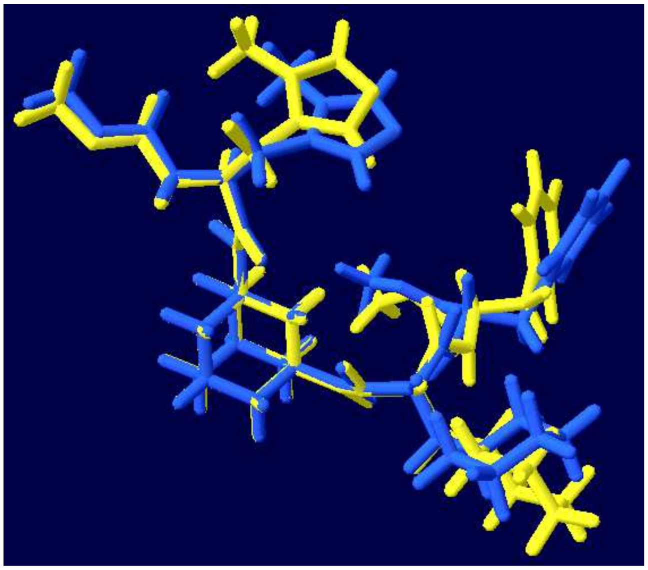
$(1R,2S)_{e,a}$-α $(1S,2R)_{a,e}$-β

Figure S1. The ONIOM2(B3LYP/6-31G*:PM3) optimized geometries of the lower energy transition states for the acylium transfer to *cis*-cyclohexane-1,2-diol. Only selected hydrogens are shown for clarity.

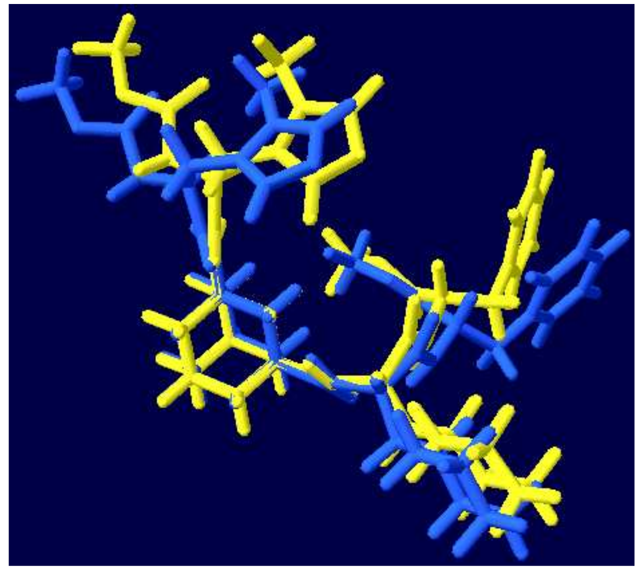


$(1R,2S)_{e,a}$-α $(1R,2S)_{e,a}$-α'

Figure S2. The ONIOM2(B3LYP/6-31G*:PM3) optimized geometries of the two possible transition states for acylium transfer to *cis*-cyclohexane-1,2-diol leading to (1*R*,2*S*) product. Only selected hydrogens are shown for clarity.

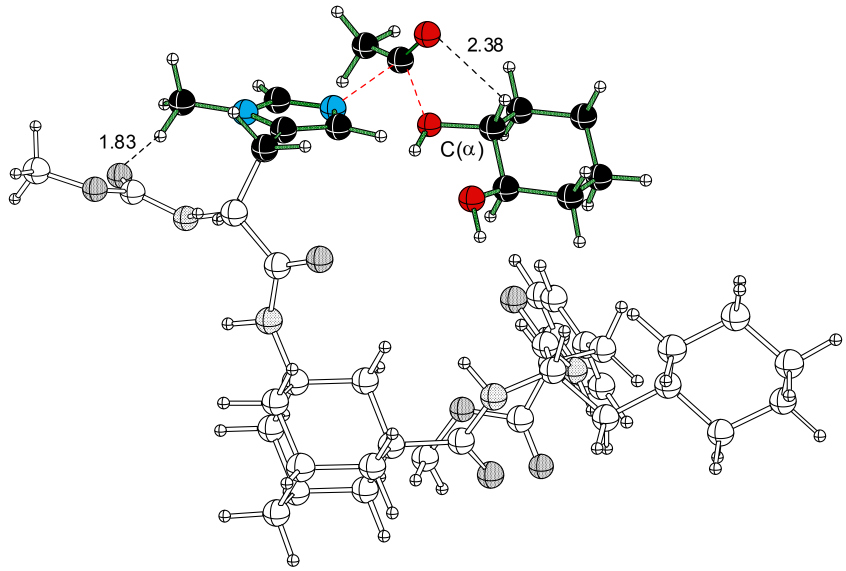


1a

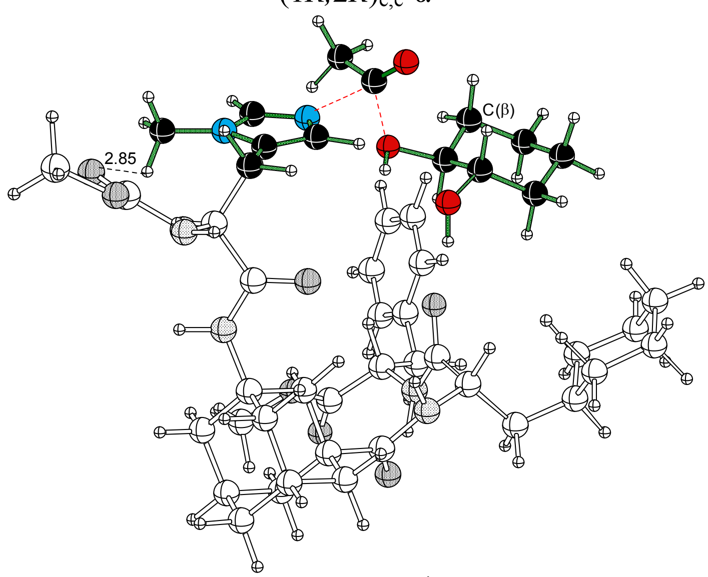


1b

Figure S3. A comparison of conformational changes of the catalyst in the diastereomeric acylation transition states for *trans*-cyclohexane-1,2-diol (**1a**, with peptide chain in TS-(1R,2R)$_{e,e}$-α in yellow and (1S,2S)$_{e,e}$-β in blue) and *cis*-cyclohexane-1,2-diol (**1b**, with peptide chain in TS-(1R,2S)$_{e,a}$-α in yellow and (1S,2R)$_{a,e}$-β in blue).



$(1R,2R)_{e,e}$-$\alpha^{\ddagger}$



$(1S,2S)_{e,e}$-$\beta^{\ddagger}$

Figure S4. The ONIOM2(B3LYP/6-31G*) optimized geometries of lower energy TSs for the acylium transfer to *trans*-diol showing the weak interactions.

Ref 9b.

Gaussian 03, Revision C.02, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004.

Table S1. Computed Relative Energies (in kcal/mol) of Transition States for the Acyl Transfer

Diol	Transition states	Relative $\Delta E^{\ddagger}$			
		Boc (**2**)		Moc (**3**)	
		L1[a]	*L2*[b]	*L1*	*L2*
Trans-diol	$(1S,2S)_{e,e}$-$\alpha^{\ddagger\ i}$	13.5	9.3	13.4	12.8
	$(1S,2S)_{e,e}$-$\beta^{\ddagger}$	4.6	4.6	4.5	4.6
	$(1S,2S)_{a,a}$-$\beta^{\ddagger}$	7.6	7.3	7.7	7.5
	$(1R,2R)_{e,e}$-$\alpha^{\ddagger}$	**0.0**	**0.0**	**0.0**	**0.0**
	$(1R,2R)_{e,e}$-$\beta^{\ddagger}$	11.5	11.2	11.6	11.1
	$(1R,2R)_{a,a}$-$\beta^{\ddagger}$	9.7	9.3	11.6	11.3
Cis-diol	**$(1R,2S)_{e,a}$-$\alpha^{\ddagger}$**	**0.0**	**0.0**	**0.0**	**0.0**
	$(1R,2S)_{e,a}$-$\beta^{\ddagger}$	16.1	15.7	16.3	15.9
	$(1R,2S)_{a,e}$-$\beta^{\ddagger}$	12.5	12.1	12.6	12.2
	$(1S,2R)_{e,a}$-$\alpha^{\ddagger}$	12.7	12.4	12.7	12.6
	$(1S,2R)_{e,a}$-$\beta^{\ddagger}$	14.9	14.6	15.0	14.7
	$(1S,2R)_{a,e}$-$\beta^{\ddagger}$	4.3	4.0	4.4	4.1

[a]*L1* : B3LYP/6-31G*//ONIOM2(B3LYP/6-31G*:PM3)
[b]*L2* : B3LYP/6-31G**//ONIOM2(B3LYP/6-31G*:PM3)

Table S2. Computed Reorganization Energies of the Pre-reacting Complexes and Activation Barriers of Transition States Obtained for the Acyl Transfer at the B3LYP/6-31G*//ONIOM2(B3LYP/6-31G*:PM3) level of theory[a]

Diol	Transition states	Moc (**3**)		
		ΔE^{b}	$\Delta E^{\ddagger c}$	$\Delta E^{\ddagger d}$
Trans-diol	$(1S,2S)_{e,e}$-$\alpha^{\ddagger\, i}$	0.9	21.8	22.7
	$(1S,2S)_{e,e}$-$\beta^{\ddagger}$	-11.6	25.4	13.8
	$(1S,2S)_{a,a}$-$\beta^{\ddagger}$	-3.2	20.2	17.1
	$(1R,2R)_{e,e}$-$\alpha^{\ddagger}$	-15.9	25.2	9.3
	$(1R,2R)_{e,e}$-$\beta^{\ddagger}$	1.0	20.0	20.9
	$(1R,2R)_{a,a}$-$\beta^{\ddagger}$	-3.5	24.4	20.9
Cis-diol	$(1R,2S)_{e,a}$-$\alpha^{\ddagger}$	-18.4	24.3	5.9
	$(1R,2S)_{e,a}$-$\beta^{\ddagger}$	3.6	18.6	22.2
	$(1R,2S)_{a,e}$-$\beta^{\ddagger}$	-6.3	24.8	18.5
	$(1S,2R)_{e,a}$-$\alpha^{\ddagger}$	0.1	18.7	18.7
	$(1S,2R)_{e,a}$-$\beta^{\ddagger}$	-3.0	23.9	20.9
	$(1S,2R)_{a,e}$-$\beta^{\ddagger}$	-11.8	22.1	10.3

[a] *In general, the reorganization of catalyst-acylium complex and diol leading the formation of inclusion complexes (as presented in the manuscript) are preferred energetically. The reaction is likely to proceed through pathways involving relatively more stabilized inclusion complex. For trans-diols, the more stabilized inclusion complex is* $(1R,2R)_{e,e}$-$\alpha^{\ddagger}$ *(by -15.9 kcal/mol). The activation barrier for this inclusion complex for acyl transfer is 9.3 kcal/mol, which is much lower than those with other complexes. Hence the reaction prefers a pathway through the formation of stabilized inclusion complexes.*

[b] *Reorganization energy associated with the formation of pre-reacting complexes (PRC) from isolated reactants, catalyst-acylium complex and diol.*

[c] *Absolute activation barrier with respect to the respective pre-reacting complex.*

[d] *Absolute activation barrier with respect to the isolated reactants, catalyst-acylium complex and diol.*

ONIOM2(B3LYP/6-31G*:PM3) optimized Cartesian coordinates for the transition states located for the acyl transfer reaction to cyclohexane-1,2-diol. Electronic energies (in a.u) at the ONIOM2(B3LYP/6-31G*:PM3) and single-point energies calculated at the B3LYP/6-31G*//ONIOM2(B3LYP/6-31G*:PM3) level of theory are given in parenthesis

Catalyst Moc-(π-Me)His-^{A}Gly-Cha-Phe-OMe

(1R,2R)e,e-α

Et= -844.665214 (-2913.1550836)

6	-1.661134	3.301105	-0.640261
6	-3.006163	3.076363	-1.338270
6	-3.932306	4.289593	-1.119819
6	-3.271660	5.612501	-1.541531
6	-1.911061	5.819083	-0.845138
6	-1.040522	4.606383	-1.119210
6	1.523587	5.493376	-1.327558
8	1.407648	5.372985	-2.485415
6	2.021576	6.546835	-0.405154
7	2.883818	3.853042	-0.659867
6	3.017385	2.650331	-1.321431
6	4.277091	2.136356	-1.119493
7	4.928010	3.073010	-0.320238
6	4.055120	4.074323	-0.075522
6	4.917601	0.875621	-1.634996
6	5.089562	-0.198679	-0.543476
7	6.320182	-1.019845	-0.726753
6	7.562774	-0.438425	-0.348285
6	3.918243	-1.206409	-0.507887
8	3.288623	-1.513067	-1.508409
7	3.576700	-1.703559	0.774765
6	2.733475	-2.928479	1.006925
6	3.300913	-4.175089	0.298071
6	2.424550	-5.388681	0.611619
6	0.999136	-5.139541	0.115635
6	0.414630	-3.906568	0.824892
6	1.292154	-2.675130	0.533230
6	2.408803	-5.639036	2.119365
6	1.831762	-4.412840	2.826862
6	0.404217	-4.165831	2.339989
6	2.704355	-3.192771	2.531381
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6	-2.295115	-2.425523	-1.530661
6	-2.350998	-1.118403	-0.717833
7	-3.430259	-0.860299	0.144660
6	-3.312199	0.089416	1.288563
6	-4.554382	0.993328	1.310524
6	-4.565204	1.923408	2.480801
6	-3.682394	3.003353	2.535760
6	-3.712729	3.880047	3.613094
6	-4.627424	3.687463	4.643465
6	-5.511126	2.614834	4.592775
6	-5.482490	1.734581	3.516088
6	-3.600354	-3.230638	-1.561398
8	-1.463973	-0.272128	-0.840560
8	7.710033	0.544706	0.370433
6	-3.153255	-0.720565	2.581869
8	-1.908442	-0.570850	3.125443
6	-1.513177	-1.409693	4.190991
8	-3.973050	-1.443166	3.104726
1	4.341452	-4.367577	0.626789
1	3.343040	-4.018637	-0.798221
1	2.841077	-6.282989	0.090803
1	3.431729	-5.851522	2.486221
1	1.805014	-6.537258	2.353729
1	2.310636	-2.309225	3.072497
1	3.727730	-3.367639	2.921489
1	1.816101	-4.591509	3.927913
1	-0.234804	-5.040886	2.572627
1	-0.053267	-3.305796	2.881928
1	1.267827	-2.456204	-0.557763
1	0.873168	-1.783786	1.042073
1	1.003557	-4.997798	-0.983178
1	0.365178	-6.026170	0.312929
1	4.328954	-1.644300	1.429193
1	5.174118	0.307736	0.453305
1	6.329792	-1.535053	-1.582625
1	5.896620	1.125036	-2.090852
1	4.291521	0.499029	-2.465317
1	2.201959	2.220689	-1.888733
1	4.315979	4.936811	0.521187
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1	-4.020598	-1.654842	0.319956
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1	-2.277267	-1.526349	4.966864
1	-1.215046	-2.393679	3.796057
1	-4.563657	1.592803	0.367522
1	-5.482361	0.385357	1.300054
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1	-3.016562	4.723991	3.650530
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1	2.113170	6.173634	0.612698
1	-2.057950	-2.149214	-2.599839
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1	-7.126600	-1.794454	-3.332648
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1	10.026829	-0.916107	0.665632
1	10.513935	-1.569692	-0.940066
1	10.179932	0.188101	-0.739443
6	6.335146	3.088923	0.071601
1	6.696257	2.070962	0.323341
1	6.950453	3.488508	-0.740258
1	6.450415	3.725607	0.950465
1	-2.048597	5.932911	0.237483
1	-1.837092	3.369657	0.451410
8	-0.648925	2.332630	-0.906576
1	-0.968825	1.427350	-0.690262

(1R,2R)$_{a,a}$-β

Et= -844.647293 (-2913.1366495)

6	-2.844712	-2.147887	-1.880130
6	-1.693937	-1.203983	-1.498501
6	-1.619836	-0.890884	0.007909
8	-1.615456	0.275162	0.434006
7	-0.388258	-1.692621	-2.019083
6	0.292000	-2.840853	-1.516121
8	-0.329384	-3.635026	-0.820135
6	1.773620	-2.980722	-1.896074
6	1.939714	-3.029519	-3.425062
6	3.426406	-3.101880	-3.778359
6	4.150654	-1.865579	-3.240184
6	4.005336	-1.809672	-1.708158
6	2.513020	-1.756794	-1.328839
6	4.034034	-4.367065	-3.174456
6	3.876554	-4.321731	-1.655183
6	2.392108	-4.251073	-1.290957
6	4.610791	-3.098818	-1.103588
7	4.743454	-0.629469	-1.139084
6	4.266331	0.702565	-1.230698
8	3.615456	1.069616	-2.196843
6	4.667411	1.654101	-0.083637
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6	6.798783	2.267200	1.046230
8	6.350915	2.167687	2.179455
6	3.910613	2.991430	-0.124295
6	2.466313	2.896892	0.288463
6	1.328925	3.216819	-0.410112
7	0.223659	3.075325	0.398317
6	0.675672	2.679664	1.580856
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6	-3.192022	1.940939	-2.575110
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6	-4.727715	3.336923	-1.043458
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8	-1.172201	4.481961	-1.407107
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1	3.735968	-0.952436	-3.711348
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1	3.539048	-5.268142	-3.586003
1	4.535911	-3.089648	0.004084
1	5.690718	-3.169366	-1.342780
1	4.316497	-5.243860	-1.207069
1	1.861970	-5.149666	-1.662909
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1	2.041025	-0.827982	-1.719026
1	2.408360	-1.732455	-0.218286
1	1.488452	-2.139281	-3.905731
1	1.405206	-3.909406	-3.833806
1	5.172458	-0.840895	-0.262654
1	4.434308	1.148099	0.897060
1	6.442414	2.294723	-0.987998
1	4.422814	3.728132	0.528368
1	3.931521	3.418293	-1.143731
1	1.239060	3.553902	-1.433500
1	0.073635	2.456303	2.451149
1	0.241077	-0.946216	-2.249965
1	-1.344597	-2.852589	0.518868
1	-1.283390	-0.658247	2.611302
1	2.825757	-2.091125	1.460720
1	2.732988	-2.286882	3.257884
1	2.213632	-3.621483	2.175792
1	-3.526577	-2.095010	2.540117
1	-2.546578	-3.403763	3.221495
1	-2.284117	0.312254	3.781204
1	-2.673437	1.370811	6.010282
1	-3.350833	-0.032272	7.949037
1	-3.642071	-2.485442	7.662425
1	-3.270567	-3.537035	5.446171
1	-1.108719	5.637467	1.102746
1	-2.829423	5.344650	0.748193
1	-1.936884	4.193465	1.771635
1	-1.860386	-0.226452	-2.037814
1	-2.865878	-3.051609	-1.236358
1	-2.648340	-2.532205	-2.904567
1	-2.201047	3.697599	-3.367475
1	-3.023219	2.719756	-4.573486
1	-4.210148	4.905233	-4.108811
1	-5.234251	3.508411	-3.792833
1	-3.713384	5.137736	-1.689125
1	-5.458321	5.133326	-1.934731
1	-4.791589	3.693650	-0.003188
1	-3.929565	1.385846	-0.623866
1	-2.250059	1.366356	-2.559556
1	-1.827021	1.923125	-0.137144
1	-3.965324	1.227032	-2.907354
1	-6.142957	1.971602	-0.801436
6	-6.529912	-1.526916	-2.853123
6	-5.158293	-2.182517	-2.843900
6	-4.219183	-1.469118	-1.867297
6	-4.838581	-1.474474	-0.468061
6	-6.222980	-0.845547	-0.463122
6	-7.143305	-1.526241	-1.462673
1	-5.247536	-3.252037	-2.566136
1	-4.728510	-2.168445	-3.865074
1	-6.450506	-0.488181	-3.233378
1	-7.195656	-2.057590	-3.560659
1	-4.901600	-2.515130	-0.088854
1	-4.181640	-0.933514	0.243086
1	-6.657336	-0.902782	0.553752
1	-6.146445	0.240535	-0.693832
1	-7.344739	-2.566790	-1.138193
1	-8.127018	-1.018896	-1.480009
1	-4.115498	-0.402959	-2.216137
8	8.041217	2.741751	0.764457
6	8.894817	3.052001	1.849703
1	9.801840	3.382049	1.336624
1	8.483854	3.857234	2.467344
1	9.097774	2.172305	2.469052
6	2.857950	2.170440	2.704551
1	3.558623	1.381734	2.402823
1	3.426523	3.030510	3.070664
1	2.218522	1.794135	3.504302

(1R,2R)e,e-β

Et= -844.654235 (−2913.1366021)

6	-2.969176	-2.775250	-2.063345
6	-1.913774	-1.760890	-1.586514
6	-2.188362	-1.195097	-0.178221
8	-2.177279	0.018706	0.033718
7	-0.532566	-2.310979	-1.677770
6	-0.030839	-3.317185	-0.804744
8	-0.829812	-3.993664	-0.167085
6	1.493839	-3.491767	-0.742792
6	2.025492	-3.987749	-2.097900
6	3.548359	-4.120553	-2.034348
6	4.177612	-2.761116	-1.722746
6	3.660186	-2.252357	-0.363236
6	2.126936	-2.128913	-0.406352
6	3.929525	-5.128200	-0.950320
6	3.407850	-4.636228	0.399153
6	4.034923	-3.281739	0.730094
6	1.886095	-4.501524	0.347928
7	4.255657	-0.932321	0.041121
6	4.178770	0.253789	-0.733495
8	3.466628	0.344018	-1.721395
6	4.974543	1.446971	-0.165213
7	6.364136	1.326683	-0.686581
6	7.394495	1.987918	0.054039
8	7.318260	2.349308	1.218143
6	4.337852	2.802173	-0.509167
6	3.000018	3.031323	0.139686
6	1.777937	3.291932	-0.429157
7	0.831274	3.497859	0.550369
6	1.470197	3.376214	1.706648
7	2.779873	3.095491	1.514721
6	-0.899233	4.722014	-0.043887
6	-1.172756	5.423702	1.233632
8	-0.672530	5.012972	-1.153060
7	-2.479203	-2.091958	0.858421
6	-2.484175	-1.675184	2.288497
6	-1.309748	-2.354165	3.002022
8	-1.303201	-3.380009	3.643842
6	-3.828025	-2.052374	2.930807
6	-4.102572	-1.272044	4.177272
6	-3.845409	0.099505	4.230164
6	-4.148758	0.827769	5.372904
6	-4.710429	0.190756	6.475086
6	-4.961734	-1.176342	6.431238
6	-4.658956	-1.908327	5.287695
8	-0.133120	-1.668035	2.831807
6	1.062571	-2.259494	3.296486
6	-2.617849	2.507514	-2.169954
6	-3.869189	2.220476	-3.018171
6	-4.779028	3.452503	-3.122766
6	-5.144500	4.001899	-1.733810
6	-3.895536	4.288488	-0.888107
6	-3.053439	3.010230	-0.794976
8	-1.907717	3.247272	0.124774
1	5.281782	-2.852010	-1.706646
1	3.935195	-2.043576	-2.531557
1	3.924274	-4.477158	-3.022324
1	5.028377	-5.260247	-0.915077
1	3.507095	-6.124590	-1.185055
1	3.681450	-2.938392	1.724671
1	5.135492	-3.391376	0.808720
1	3.682064	-5.369529	1.194005
1	1.418807	-5.485437	0.147090
1	1.497424	-4.170460	1.338353
1	1.815294	-1.377976	-1.165876
1	1.745747	-1.768670	0.572370
1	1.742925	-3.290744	-2.911373
1	1.567069	-4.964137	-2.349797
1	5.136337	-1.040815	0.499984
1	5.025613	1.357268	0.958030
1	6.415948	1.440709	-1.677755
1	5.030640	3.619098	-0.219646
1	4.190650	2.895481	-1.600965
1	1.528904	3.354799	-1.479833
1	1.033058	3.477850	2.690288
1	0.153831	-1.616452	-1.906705
1	-2.189990	-3.048068	0.677474
1	-2.368795	-0.555455	2.365194
1	1.810857	-1.497153	3.061344
1	1.039916	-2.457377	4.373121
1	1.286128	-3.187907	2.745376
1	-4.655410	-1.850827	2.218701
1	-3.869964	-3.141941	3.138775
1	-3.385060	0.585676	3.357435
1	-3.946501	1.902847	5.406314
1	-4.952273	0.764461	7.375946
1	-5.399167	-1.680498	7.299884
1	-4.855938	-2.986862	5.261290
1	-3.628410	2.234054	-0.271607
1	-5.773644	3.272421	-1.200405
1	-5.724853	4.926740	-1.812511
1	-5.691492	3.200714	-3.673343
1	-4.270911	4.236080	-3.701014
1	-4.424183	1.379901	-2.561361
1	-3.573122	1.867589	-4.018664
1	-1.268090	2.507702	0.071640
1	-0.482051	6.266251	1.315227
1	-2.210155	5.774983	1.184859
1	-1.076594	4.751856	2.083372
1	-1.917661	-0.895905	-2.312623
1	-3.688954	-3.007781	-1.252171
1	-2.483638	-3.744033	-2.305534
6	-3.765504	-2.326974	-3.292776
6	-2.860179	-1.844793	-4.425586
1	-4.324658	-3.225279	-3.659447
6	-3.671455	-1.448104	-5.647675
1	-2.253891	-0.980749	-4.068777
1	-2.133686	-2.636895	-4.690929
6	-4.702742	-0.388219	-5.298636
1	-2.997474	-1.076529	-6.443356
1	-4.175839	-2.339996	-6.070668
6	-5.607788	-0.861356	-4.171637
1	-4.190712	0.556598	-5.000545
1	-5.306535	-0.135394	-6.190813
6	-4.799521	-1.256692	-2.944642
1	-6.327285	-0.062900	-3.904132
1	-6.219759	-1.719511	-4.514022
1	-4.301414	-0.354679	-2.519673
1	-5.475681	-1.628282	-2.150041
8	8.519964	2.101808	-0.700720
6	9.691598	2.589562	-0.074412
1	10.415513	2.557550	-0.892792
1	9.558319	3.614980	0.285527
1	10.008902	1.942410	0.749723
6	3.783515	2.957930	2.569698
1	4.362432	2.038035	2.420198
1	4.465818	3.813268	2.562841
1	3.278875	2.908056	3.535625
1	-2.020471	1.589493	-2.061938
1	-1.987379	3.260596	-2.655977
1	-3.304598	5.063738	-1.387699
8	-4.198346	4.833863	0.390259
1	-4.875281	4.280868	0.814263

(1R,2S)e,a-α
Et=-844.664357 (−2913.160383)

6	-3.194343	2.617402	-0.577159
6	-4.574828	2.347749	0.031160
6	-4.977738	3.374259	1.098079
6	-4.855105	4.806797	0.564763
6	-3.413287	5.093384	0.110518
6	-2.974048	4.095269	-0.956467
6	-0.845341	3.952211	-2.624388
8	-1.110016	2.910690	-3.105019
6	-0.559435	5.298811	-3.199774
7	1.089879	3.665280	-1.589835
6	1.931943	2.693082	-2.074588
6	3.185612	2.837895	-1.526025
7	3.086829	3.941032	-0.681980
6	1.816694	4.400780	-0.758779
6	4.459456	2.071180	-1.764568
6	4.763960	1.050604	-0.649606
7	6.222003	0.932125	-0.367137
6	6.835591	1.968694	0.387113
6	4.243526	-0.367346	-0.980203
8	3.797058	-0.668594	-2.078130
7	4.372059	-1.330613	0.043167
6	3.667038	-2.658572	0.063420
6	4.246187	-3.596154	-1.014238
6	3.554025	-4.958484	-0.936852
6	2.052080	-4.794333	-1.177988
6	1.456213	-3.870269	-0.102794
6	2.151457	-2.496847	-0.154024
6	3.789468	-5.580825	0.438601
6	3.201738	-4.663738	1.510065
6	1.699215	-4.498731	1.278570
6	3.889470	-3.298726	1.454228
6	-0.041796	-3.644019	-0.354073
8	-0.933851	-3.987930	0.412625
7	-0.404432	-2.981683	-1.563210
6	-1.685775	-2.242548	-1.719830
6	-1.879412	-1.228332	-0.576179
7	-2.331113	-1.677895	0.667495
6	-2.271939	-0.818549	1.888324
6	-3.698081	-0.556594	2.399765
6	-3.705072	0.193600	3.693530
6	-3.457585	1.567057	3.715623
6	-3.476639	2.262360	4.918719
6	-3.750870	1.594262	6.107594
6	-4.010228	0.228073	6.089250
6	-3.988900	-0.471961	4.887640
6	-2.880778	-3.185254	-1.911330
8	-1.657885	-0.025926	-0.757396
8	6.253817	2.804997	1.071286
6	-1.393945	-1.539156	2.917354
8	-0.112065	-1.054283	2.920693
6	0.855274	-1.707605	3.716176
8	-1.688103	-2.458632	3.647275
1	5.337926	-3.718197	-0.870431
1	4.112172	-3.166722	-2.026830
1	3.977438	-5.626123	-1.723987
1	4.872268	-5.733951	0.612543
1	3.323485	-6.583883	0.493764
1	3.483197	-2.647980	2.257827
1	4.971896	-3.415027	1.661246
1	3.367321	-5.113920	2.517363
1	1.188891	-5.479470	1.347676
1	1.255936	-3.864864	2.079998
1	1.947775	-2.017049	-1.137481
1	1.721885	-1.829977	0.621723
1	1.879678	-4.386053	-2.193363
1	1.549017	-5.780740	-1.148799
1	4.520085	-0.950491	0.953779
1	4.267663	1.389432	0.296645
1	6.752651	0.581669	-1.136904
1	5.298136	2.786291	-1.876943
1	4.367572	1.567711	-2.745131
1	1.589551	1.949203	-2.781771
1	1.468158	5.258255	-0.200083
1	0.368482	-2.497765	-1.981386
1	-2.210839	-2.676220	0.817968
1	-1.810301	0.178349	1.637598
1	1.746453	-1.095255	3.553161
1	0.583868	-1.720233	4.776688
1	1.031555	-2.734103	3.356863
1	-4.247926	0.038045	1.628968
1	-4.255542	-1.509071	2.510259
1	-3.268545	2.108082	2.774683
1	-3.280542	3.339527	4.928239
1	-3.766848	2.143663	7.054890
1	-4.232277	-0.300479	7.022788
1	-4.187793	-1.551073	4.880190
1	-5.309403	2.345630	-0.785644
1	-5.137760	5.532172	1.334403
1	-5.549809	4.954665	-0.274104
1	-4.327384	3.247421	1.980462
1	-6.002258	3.174655	1.428498
1	0.140429	5.174928	-4.028555
1	-1.499051	5.704356	-3.595230
1	-0.154095	5.979607	-2.455337
1	-1.586268	-1.658393	-2.682239
1	-3.195818	-3.655740	-0.957303
1	-2.581605	-4.031162	-2.565489
1	-4.568929	1.327360	0.454857
6	-4.911746	-1.273319	-4.591836
6	-3.738490	-2.013441	-3.972202
6	-4.063969	-2.448510	-2.542159
6	-5.307532	-3.337256	-2.543177
6	-6.487616	-2.610179	-3.169734
6	-6.161948	-2.139748	-4.578834
1	-3.482017	-2.898974	-4.588261
1	-2.825228	-1.377449	-3.963162
1	-5.098352	-0.329575	-4.041509
1	-4.665611	-0.975171	-5.628948
1	-5.099651	-4.274961	-3.096913
1	-5.557590	-3.644815	-1.508909
1	-7.371932	-3.275854	-3.187932
1	-6.774458	-1.744321	-2.539910
1	-6.019215	-3.014663	-5.244137
1	-7.017924	-1.577308	-4.998480
1	-4.284337	-1.535364	-1.934153
1	-3.415095	4.315683	-1.931054
8	-1.493225	4.242469	-1.109533
1	-1.171010	3.488677	-0.513312
1	-3.307722	6.111971	-0.277634
8	8.188437	1.877834	0.313834
6	8.959651	2.730438	1.139526
1	8.755550	2.558535	2.201327
1	9.979022	2.427275	0.886652
1	8.796105	3.784564	0.892965
6	4.163281	4.573694	0.073979
1	4.814043	3.812799	0.551364
1	4.773902	5.200699	-0.582617
1	3.727014	5.199257	0.854519
1	-2.740437	5.000166	0.971612
1	-3.050095	2.003027	-1.473907
8	-2.116786	2.351459	0.349876
1	-1.873674	1.391681	0.289633

(1R,2S)e,a-β
Et= -844.660074 (-2913.1344125)

6	-2.518285	-3.700473	-1.376393
6	-1.532970	-2.526690	-1.265344
6	-1.813825	-1.563181	-0.096678
8	-1.833617	-0.343701	-0.266697
7	-0.119077	-2.995998	-1.218047
6	0.443937	-3.632680	-0.074282
8	-0.310654	-4.139775	0.748066
6	1.975453	-3.632854	0.040790
6	2.608840	-4.390022	-1.138422
6	4.133798	-4.327420	-1.028509
6	4.600346	-2.870549	-1.065337
6	3.979576	-2.099165	0.115743
6	2.445292	-2.166161	0.027112
6	4.580312	-4.980912	0.278809
6	3.955702	-4.229926	1.453996
6	4.419834	-2.773090	1.437663
6	2.431361	-4.289356	1.353492
7	4.414055	-0.660834	0.177316
6	4.238953	0.274546	-0.874922
8	3.548724	0.034015	-1.853043
6	4.898240	1.648970	-0.636695
7	6.316609	1.525803	-1.075052
6	7.248458	2.464621	-0.530730
8	7.086290	3.129185	0.481322
6	4.164391	2.792575	-1.354460
6	2.820321	3.123910	-0.765237
6	1.574373	3.114471	-1.343747
7	0.630549	3.568689	-0.449213
6	1.292435	3.859814	0.662659
7	2.615786	3.610906	0.524541
6	-1.263258	4.326214	-1.361762
6	-1.463036	5.543023	-0.546256
8	-1.164591	4.012469	-2.475704
7	-2.061960	-2.096726	1.177960
6	-2.112744	-1.226901	2.387332
6	-1.030446	-1.683923	3.370548
8	-1.130261	-2.425442	4.321961
6	-3.521732	-1.277917	3.008437
6	-3.920876	0.064586	3.532996
6	-4.161789	1.112675	2.642664
6	-4.537315	2.363818	3.115319
6	-4.686657	2.576916	4.481423
6	-4.455190	1.533732	5.372270
6	-4.071212	0.281229	4.903077
8	0.193666	-1.146930	3.063599
6	1.333780	-1.616501	3.752210
6	-3.426038	1.869448	-2.099162
6	-4.761204	1.137077	-2.314973
6	-5.957577	2.049835	-2.013100
6	-5.862822	2.647435	-0.600290
6	-4.522226	3.360378	-0.346731
6	-3.384697	2.393676	-0.666557
8	-2.097709	3.036685	-0.299457
1	5.706454	-2.828098	-1.016292
1	4.312749	-2.411124	-2.031806
1	4.583537	-4.874814	-1.890309
1	5.684793	-4.972365	0.357489
1	4.278489	-6.046181	0.299689
1	3.993524	-2.234435	2.309599
1	5.521938	-2.733581	1.552887
1	4.276324	-4.704259	2.411535
1	2.082810	-5.339725	1.398107
1	1.969555	-3.773716	2.226755
1	2.082538	-1.673203	-0.902144
1	1.990337	-1.617281	0.878131
1	2.286724	-3.959114	-2.106885
1	2.268434	-5.444081	-1.137623
1	5.282796	-0.549553	0.657498
1	4.904335	1.871518	0.468854
1	6.404688	1.364160	-2.056987
1	4.799591	3.702371	-1.345507
1	4.002169	2.541843	-2.419013
1	1.304255	2.814457	-2.347409
1	0.862653	4.240215	1.579090
1	0.517008	-2.349084	-1.646190
1	-1.709612	-3.039103	1.312648
1	-1.896336	-0.164812	2.091961
1	2.124348	-0.964825	3.367825
1	1.244414	-1.514674	4.838633
1	1.548155	-2.663218	3.483425
1	-4.268924	-1.592314	2.249710
1	-3.578666	-2.043720	3.809409
1	-4.055176	0.947817	1.558055
1	-4.716392	3.177917	2.396022
1	-4.990487	3.560456	4.854628
1	-4.577513	1.696984	6.448731
1	-3.890177	-0.537220	5.610822
1	-3.466015	1.556625	0.049072
1	-5.973074	1.855717	0.154841
1	-6.680412	3.356954	-0.414915
1	-6.894705	1.491688	-2.113148
1	-5.990667	2.860206	-2.751978
1	-4.791223	0.238867	-1.667522
1	-4.813556	0.755437	-3.346803
1	-1.391743	2.360101	-0.279658
1	-0.808736	6.323856	-0.942060
1	-2.515653	5.817750	-0.674093
1	-1.258568	5.354967	0.504263
1	-1.615056	-1.935039	-2.223573
1	-2.897728	-4.009400	-0.381201
1	-1.978685	-4.589025	-1.768439
6	-3.712294	-3.442897	-2.298903
6	-3.274344	-3.021370	-3.701428
1	-4.256021	-4.418249	-2.390251
6	-4.472083	-2.845171	-4.620258
1	-2.686141	-2.077686	-3.637083
1	-2.582908	-3.776881	-4.123199
6	-5.481969	-1.868267	-4.041645
1	-4.134529	-2.496663	-5.615293
1	-4.957820	-3.826763	-4.792557
6	-5.905254	-2.280724	-2.640008
1	-5.051452	-0.840032	-4.015610
1	-6.367929	-1.804872	-4.702003
6	-4.698019	-2.426945	-1.724886
1	-6.604088	-1.529684	-2.221197
1	-6.470280	-3.233160	-2.679077
1	-4.213332	-1.431293	-1.591429
1	-5.021394	-2.742591	-0.713742
8	8.394802	2.471160	-1.262304
6	9.488303	3.225689	-0.774859
1	10.250862	3.035652	-1.534607
1	9.249666	4.293031	-0.723563
1	9.820446	2.869464	0.205689
6	3.639460	3.864372	1.537313
1	4.269645	2.975128	1.665121
1	4.270878	4.708208	1.242977
1	3.151629	4.094449	2.485639
1	-2.584858	1.184750	-2.271253
1	-4.455212	3.643397	0.722655
1	-3.332667	2.700295	-2.802806
8	-4.350941	4.513257	-1.175901
1	-5.177227	5.021817	-1.165511

(1R,2S)$_{a,c}$-β

Et=-844.650323 (-2913.140336)

6	-2.813335	-2.364847	-1.805975
6	-1.680410	-1.390371	-1.446697
6	-1.677583	-0.957585	0.032145
8	-1.685912	0.238009	0.360454
7	-0.352595	-1.910997	-1.868355
6	0.309431	-3.009261	-1.245550
8	-0.336982	-3.744956	-0.509378
6	1.802985	-3.174925	-1.563557
6	2.011866	-3.379987	-3.074335
6	3.507931	-3.478746	-3.377650
6	4.211795	-2.188522	-2.950950
6	4.023904	-1.975380	-1.437392
6	2.521695	-1.893871	-1.105801
6	4.103660	-4.670290	-2.629308
6	3.903499	-4.469247	-1.127746
6	2.409091	-4.371817	-0.813871
6	4.616912	-3.190756	-0.685625
7	4.743040	-0.737985	-0.976313
6	4.270955	0.576025	-1.218820
8	3.626996	0.836331	-2.223690
6	4.672629	1.646923	-0.182785
7	6.143083	1.851598	-0.296165
6	6.812031	2.408727	0.835630
8	6.386811	2.419882	1.981770
6	3.892176	2.961070	-0.346351
6	2.455096	2.889896	0.095397
6	1.304845	3.147363	-0.608612
7	0.211686	3.067262	0.224483
6	0.684572	2.770889	1.426764
7	2.033010	2.650441	1.403242
6	-1.521292	4.138999	-0.492185
8	-2.481143	2.635538	-0.458847
6	-3.588608	2.212872	-1.355623
6	-3.122365	1.724217	-2.733663
6	-2.916642	2.819268	-3.788103
6	-4.127983	3.759058	-3.862846
6	-4.433209	4.379223	-2.491076
6	-4.680559	3.301913	-1.433953
7	-1.688616	-1.937764	1.016068
6	-1.533405	-1.634325	2.465601
6	-0.232777	-2.260057	2.978125
8	-0.073559	-3.107406	3.825286
6	-2.764453	-2.147922	3.230045
6	-2.976150	-1.426927	4.523670
6	-2.835756	-0.039562	4.598252
6	-3.083004	0.628757	5.790072
6	-3.469981	-0.084916	6.920210
6	-3.602912	-1.467687	6.854420
6	-3.356613	-2.139646	5.661441
8	0.867509	-1.735053	2.344428
6	2.132138	-2.322141	2.568249
6	-1.954382	4.799813	0.765261
8	-1.209004	4.490411	-1.564330
1	5.290109	-2.244972	-3.199110
1	3.806428	-1.331727	-3.524887
1	3.647530	-3.622192	-4.475180
1	5.180720	-4.774087	-2.864734
1	3.624140	-5.612560	-2.958695
1	4.509765	-3.067069	0.412478
1	5.703528	-3.278563	-0.885538
1	4.334554	-5.337007	-0.574715
1	1.893391	-5.307641	-1.105772
1	2.252149	-4.261053	0.278808
1	2.057696	-1.012739	-1.602019
1	2.385231	-1.755906	-0.007145
1	1.570403	-2.546724	-3.655720
1	1.492106	-4.300708	-3.404626
1	5.159539	-0.855559	-0.076617
1	4.466920	1.241446	0.849182
1	6.419766	2.217740	-1.183094
1	4.401696	3.767377	0.220825
1	3.892578	3.283421	-1.403797
1	1.200059	3.403869	-1.653772
1	0.098374	2.620383	2.323045
1	0.282770	-1.182889	-2.138282
1	-1.426820	-2.869670	0.709767
1	-1.470229	-0.518071	2.620625
1	2.711729	-1.942572	1.713769
1	2.555557	-1.978047	3.516354
1	2.110663	-3.418630	2.542897
1	-3.677347	-2.005950	2.612837
1	-2.686575	-3.240965	3.405528
1	-2.512774	0.510148	3.702024
1	-2.974441	1.716776	5.840406
1	-3.667058	0.441315	7.860287
1	-3.901422	-2.031861	7.744867
1	-3.457942	-3.230777	5.618424
1	-1.311641	5.667416	0.929776
1	-2.995462	5.106778	0.617886
1	-1.909415	4.117835	1.611486
1	-1.821115	-0.459175	-2.068219
1	-2.932106	-3.159975	-1.041479
1	-2.530381	-2.903554	-2.736163
1	-2.018132	3.398557	-3.550882
1	-2.740462	2.343993	-4.759213
1	-3.944834	4.553989	-4.593146
1	-5.006651	3.203913	-4.220893
1	-3.602824	5.022855	-2.181284
1	-5.324466	5.013208	-2.533617
1	-3.996980	1.358619	-0.795059
1	-2.209362	1.117322	-2.608682
1	-1.864122	1.870131	-0.300923
1	-3.895139	1.010363	-3.074089
6	-6.351734	-1.790841	-3.246520
6	-5.026802	-2.489346	-2.983408
6	-4.153431	-1.660129	-2.038420
6	-4.907600	-1.421327	-0.729408
6	-6.231959	-0.718231	-0.986039
6	-7.095298	-1.516921	-1.949201
1	-5.203300	-3.493438	-2.548109
1	-4.496699	-2.662138	-3.940874
1	-6.175507	-0.840144	-3.789520
1	-6.976687	-2.410487	-3.918003
1	-5.087121	-2.386718	-0.213729
1	-4.287532	-0.819710	-0.034233
1	-6.769435	-0.565442	-0.030517
1	-6.047277	0.298239	-1.394941
1	-7.396607	-2.473743	-1.477753
1	-8.036523	-0.972709	-2.157037
1	-3.970890	-0.662772	-2.529356
8	8.039906	2.873106	0.481667
6	8.906181	3.309878	1.511872
1	9.797321	3.600914	0.949714
1	8.490317	4.167564	2.050595
1	9.137438	2.503241	2.215085
6	2.883952	2.376278	2.560786
1	3.582070	1.562991	2.326479
1	3.456025	3.267174	2.837074
1	2.255772	2.076851	3.400957
1	-5.587488	2.748733	-1.731634
8	-4.888197	3.949764	-0.184541
1	-5.246846	3.308372	0.449817

(1*S*,2*R*)$_{e,a}$-α

Et=-844.650526 (-2913.139999)

6	3.335218	-2.452252	-0.502158
6	4.748053	-2.201641	0.063384
6	5.182360	-3.313496	1.030230
6	5.050914	-4.701469	0.386679
6	3.640618	-4.958096	-0.166113
6	3.250445	-3.836615	-1.131983
6	1.200364	-3.447008	-3.063979
8	1.438206	-2.317619	-3.220757
6	0.957752	-4.631780	-3.927835
7	-0.774006	-3.492961	-1.944753
6	-1.599568	-2.445373	-2.283428
6	-2.894399	-2.720444	-1.908848
7	-2.839977	-3.978762	-1.316901
6	-1.556976	-4.400792	-1.370015
6	-4.170277	-1.945802	-2.114626
6	-4.543143	-1.067796	-0.903424
7	-6.008200	-1.056436	-0.633279
6	-6.585038	-2.207643	-0.034107
6	-4.094448	0.402474	-1.080623
8	-3.610395	0.821489	-2.122925
7	-4.336632	1.265675	0.008435
6	-3.719975	2.627848	0.173723
6	-4.296807	3.616151	-0.858890
6	-3.698711	5.006083	-0.629926
6	-2.177796	4.952729	-0.789306
6	-1.585635	3.977133	0.241556
6	-2.187778	2.574921	0.035080
6	-4.051288	5.496624	0.773418
6	-3.467076	4.529606	1.801907
6	-1.946439	4.472785	1.650835
6	-4.062406	3.136233	1.594281
6	-0.064269	3.848861	0.069151
8	0.753496	4.109395	0.943298
7	0.408540	3.382006	-1.192966
6	1.733952	2.724421	-1.359141
6	1.872022	1.525015	-0.401128
7	2.181573	1.768557	0.953177
6	1.947485	0.720071	1.989527
6	3.289797	0.216735	2.541800
6	3.096341	-0.894413	3.524719
6	2.601220	-2.129627	3.100845
6	2.443935	-3.169757	4.008515
6	2.776361	-2.985096	5.346738
6	3.269421	-1.756850	5.773628
6	3.430843	-0.713552	4.867532
6	2.896191	3.721018	-1.274971
8	1.734797	0.371512	-0.798632
8	-5.978350	-3.110664	0.534032
6	1.078515	1.323258	3.098502
8	-0.234042	0.945981	2.982878
6	-1.184029	1.522856	3.854087
8	1.408726	2.066748	3.995164
1	-5.400461	3.660918	-0.773393
1	-4.078124	3.282339	-1.892481
1	-4.118827	5.710676	-1.385991
1	-5.149746	5.570306	0.892102
1	-3.654333	6.517392	0.936910
1	-3.663198	2.445814	2.367880
1	-5.160232	3.171407	1.741257
1	-3.717728	4.883096	2.829971
1	-1.503843	5.472445	1.828776
1	-1.510335	3.801767	2.425799
1	-1.897952	2.197458	-0.970877
1	-1.759532	1.869602	0.777054
1	-1.923869	4.645825	-1.823075
1	-1.741825	5.961131	-0.648053
1	-4.493640	0.799097	0.876412
1	-4.040370	-1.477859	0.010258
1	-6.547336	-0.625441	-1.354781
1	-4.988188	-2.653537	-2.351667
1	-4.044131	-1.328449	-3.024099
1	-1.218267	-1.559861	-2.774937
1	-1.240832	-5.359380	-0.981733
1	-0.310303	2.913870	-1.712733
1	1.993794	2.722014	1.246952
1	1.412702	-0.156782	1.533658
1	-2.100251	0.986058	3.591681
1	-0.936721	1.369110	4.909479
1	-1.302327	2.597512	3.643332
1	3.920917	-0.160111	1.700456
1	3.859811	1.049107	3.002556
1	2.342061	-2.280586	2.039632
1	2.057821	-4.135727	3.665987
1	2.649641	-3.804335	6.062251
1	3.531164	-1.607890	6.826978
1	3.815593	0.254884	5.211042
1	5.467857	-2.118319	-0.762483
1	5.299908	-5.494663	1.104000
1	5.767416	-4.806080	-0.439985
1	4.559078	-3.269138	1.935297
1	6.216836	-3.152708	1.351077
1	0.260438	-4.337146	-4.715693
1	1.915618	-4.909196	-4.384652
1	0.566332	-5.471190	-3.360088
1	1.738083	2.322358	-2.415003
1	3.121830	4.006959	-0.227147
1	2.609509	4.668005	-1.778693
1	4.742229	-1.228672	0.581113
6	5.200199	2.420242	-4.097716
6	3.953182	2.991898	-3.444742
6	4.153305	3.152989	-1.936724
6	5.353621	4.060848	-1.669447
6	6.607198	3.503171	-2.326168
6	6.406357	3.304660	-3.820556
1	3.702465	3.971132	-3.900445
1	3.071369	2.338510	-3.629060
1	5.388215	1.394318	-3.723071
1	5.043976	2.320184	-5.188880
1	5.145966	5.081472	-2.049341
1	5.513809	4.169870	-0.578913
1	7.460606	4.184903	-2.146301
1	6.884500	2.540412	-1.852009
1	6.273426	4.287045	-4.316209
1	7.314751	2.859682	-4.269914
1	4.367306	2.146840	-1.496637
1	3.854039	-3.904305	-2.041217
8	1.872063	-4.161854	-1.593119
1	1.228579	-3.927833	-0.892172
1	3.071493	-1.685839	-1.238024
1	3.615684	-5.917101	-0.704949
1	2.607693	-2.389149	0.326010
8	2.624152	-4.940889	0.838504
1	2.898351	-5.506458	1.577531
8	-7.940232	-2.154979	-0.107656
6	-8.684572	-3.136057	0.589854
1	-8.491372	-3.100759	1.666919
1	-9.712912	-2.837111	0.370483
1	-8.482980	-4.141582	0.206437
6	-3.960312	-4.750629	-0.789254
1	-4.617977	-4.109778	-0.166781
1	-4.547463	-5.180991	-1.605777
1	-3.570601	-5.559697	-0.169597

(1*S*,2*R*)$_{e,a}$-β

Et= -844.658171(-2913.1365314)

6	2.656701	3.517742	-1.338983
6	1.640364	2.369274	-1.260881
6	1.831627	1.434762	-0.051742
8	1.866092	0.210657	-0.196863
7	0.234927	2.867115	-1.309473
6	-0.369137	3.570411	-0.225649
8	0.359152	4.098603	0.606933
6	-1.903783	3.609421	-0.178726
6	-2.471937	4.308346	-1.424925
6	-4.001376	4.285878	-1.372968
6	-4.503181	2.840341	-1.341674
6	-3.946809	2.127085	-0.093747
6	-2.408099	2.155388	-0.127541
6	-4.482052	5.027534	-0.126349
6	-3.923933	4.333833	1.115409
6	-4.423320	2.889671	1.165767
6	-2.395938	4.351225	1.074682
7	-4.409108	0.702360	0.040104
6	-4.239238	-0.290794	-0.956010
8	-3.552264	-0.099883	-1.948042
6	-4.888080	-1.654400	-0.637755
7	-6.345712	-1.518441	-0.913800
6	-7.222305	-2.428611	-0.243007
8	-6.957431	-3.068644	0.762897
6	-4.251231	-2.808170	-1.429040
6	-2.858364	-3.145126	-0.972784
6	-1.657052	-3.036687	-1.628432
7	-0.636474	-3.519272	-0.840796
6	-1.207384	-3.922135	0.285779
7	-2.547550	-3.715511	0.258265
6	1.323437	-3.632444	-2.044968
6	1.568355	-5.087547	-1.955889
8	1.110126	-2.811605	-2.838449
7	1.977977	1.996052	1.222937
6	1.897935	1.167216	2.459103
6	0.790397	1.731763	3.355024
8	0.876106	2.554118	4.239128
6	3.261243	1.149529	3.176159
6	3.508856	-0.186230	3.801040
6	3.719604	-1.298376	2.984345
6	3.951657	-2.548657	3.542833
6	3.984427	-2.697171	4.925313
6	3.782595	-1.590485	5.744010
6	3.543569	-0.337557	5.187240
8	-0.434129	1.198650	3.047449
6	-1.584108	1.741278	3.662622
6	3.953464	-1.961334	-1.820180
6	5.338127	-1.318859	-1.663463
6	6.346151	-2.296721	-1.042531
6	5.830392	-2.880933	0.281750
6	4.417719	-3.494528	0.150966
6	3.484081	-2.453963	-0.455153
8	2.090879	-2.995086	-0.506078
1	-5.611016	2.826395	-1.332905
1	-4.191941	2.319369	-2.268656
1	-4.403311	4.789960	-2.283450
1	-5.588632	5.049604	-0.092564
1	-4.153892	6.084771	-0.156096
1	-4.047576	2.395503	2.086181
1	-5.529940	2.881878	1.235601
1	-4.269934	4.871791	2.029533
1	-2.022088	5.393752	1.074790
1	-1.984841	3.874947	1.994479
1	-2.023421	1.601948	-1.012802
1	-1.999027	1.646151	0.770139
1	-2.122886	3.812865	-2.352267
1	-2.106513	5.352871	-1.472704
1	-5.271921	0.622185	0.536332
1	-4.764373	-1.874781	0.462070
1	-6.542022	-1.383746	-1.884028
1	-4.892627	-3.709938	-1.355252
1	-4.195042	-2.556977	-2.504228
1	-1.470134	-2.627978	-2.612429
1	-0.699684	-4.353481	1.137628
1	-0.393538	2.210124	-1.733214
1	1.662133	2.957911	1.300355
1	1.631027	0.111936	2.181060
1	-2.376339	1.077313	3.304066
1	-1.529142	1.720540	4.755904
1	-1.765198	2.769141	3.308972
1	4.080438	1.357694	2.456426
1	3.325777	1.956398	3.935034
1	3.705875	-1.182301	1.888418
1	4.114263	-3.409740	2.875601
1	4.173700	-3.680735	5.367929
1	3.813551	-1.703924	6.833319
1	3.385521	0.530934	5.838395
1	3.417351	-1.594139	0.231168
1	5.800999	-2.091227	1.047906
1	6.518695	-3.646337	0.654971
1	7.303769	-1.790904	-0.880685
1	6.531437	-3.111026	-1.752443
1	5.223489	-0.401599	-1.053224
1	5.679448	-0.964165	-2.651546
1	1.454115	-2.280529	-0.305530
1	0.866190	-5.586576	-2.628274
1	2.594687	-5.250360	-2.301498
1	1.448268	-5.445230	-0.937095
1	1.770559	1.750853	-2.196352
1	2.938882	3.881345	-0.329668
1	2.173480	4.387136	-1.834449
6	3.933102	3.198452	-2.119873
6	3.639979	2.656100	-3.517965
1	4.470831	4.174716	-2.240086
6	4.924482	2.465665	-4.308528
1	3.077015	1.698879	-3.431728
1	2.965982	3.349639	-4.058306
6	5.926729	1.596942	-3.566451
1	4.695454	2.019909	-5.295655
1	5.377622	3.454829	-4.522244
6	6.184006	2.118019	-2.160467
1	5.560922	0.545571	-3.512001
1	6.876951	1.551428	-4.132612
6	4.882408	2.254863	-1.382332
1	6.872355	1.434184	-1.625310
1	6.704402	3.095311	-2.207186
1	4.432647	1.243531	-1.241314
1	5.083993	2.638425	-0.363155
8	-8.443125	-2.436828	-0.842530
6	-9.484262	-3.162926	-0.216886
1	-10.324286	-2.981541	-0.892358
1	-9.253588	-4.231919	-0.163496
1	-9.701389	-2.777035	0.784428
6	-3.493956	-4.038568	1.323454
1	-4.155582	-3.180108	1.501475
1	-4.102269	-4.906638	1.052065
1	-2.941572	-4.259677	2.238056
1	3.238217	-1.220318	-2.209994
1	4.044991	-3.784713	1.147123
1	4.447605	-4.387655	-0.480974
8	3.987868	-3.113311	-2.671139
1	4.191272	-2.817019	-3.572323

$(1S,2R)_{a,e}$-β

Et= -844.662260 (-2913.153392)

6	-6.086774	2.791264	-3.812582
6	-4.791116	3.103827	-3.080494
6	-3.817772	1.942076	-3.190924
6	-4.438803	0.660043	-2.633489
6	-5.721806	0.339141	-3.399286
6	-6.704534	1.496837	-3.306309
6	-3.452620	-0.507279	-2.715403
6	-2.279888	-0.291548	-1.748419
6	-2.663530	-0.566511	-0.280291
8	-2.509509	0.296250	0.595202
7	-1.059001	-1.025699	-2.170170
6	-0.869593	-2.425887	-2.015325
8	-1.855775	-3.133115	-1.841080
6	0.569024	-2.955978	-2.126836
6	1.033806	-2.854853	-3.589714
6	2.470013	-3.366615	-3.710597
6	3.396693	-2.514946	-2.841991
6	2.952798	-2.603704	-1.368515
6	1.498268	-2.119450	-1.226713
6	2.536957	-4.825986	-3.262127
6	2.086540	-4.924514	-1.805123
6	0.647332	-4.424706	-1.677942
6	3.011197	-4.084458	-0.922784
7	3.831288	-1.807542	-0.441233
6	4.142711	-0.436406	-0.625620
8	3.507562	0.267578	-1.395909
6	5.245847	0.121841	0.297370
7	6.535261	-0.488197	-0.136343
6	7.579958	-0.563083	0.839082
8	7.435658	-0.493423	2.049748
6	5.312882	1.657962	0.296397
6	4.170286	2.321761	1.014899
6	3.215879	3.191070	0.546306
7	2.404910	3.601569	1.578150
6	2.857071	2.998071	2.668588
7	3.922891	2.213339	2.381870
7	-3.245884	-1.787045	0.056420
6	-3.394893	-2.236055	1.469690
6	-2.288468	-3.242361	1.805684
8	-2.380941	-4.405258	2.125505
6	-4.796150	-2.835323	1.666494
6	-5.237820	-2.802998	3.095614
6	-5.012428	-1.674774	3.887041
6	-5.470886	-1.632731	5.197153
6	-6.156941	-2.720126	5.729235
6	-6.377088	-3.849682	4.948585
6	-5.919309	-3.894373	3.635779
8	8.774651	-0.798055	0.233523
8	-1.038995	-2.682116	1.702118
6	0.092719	-3.519797	1.792781
6	1.099021	5.282022	1.094876
8	1.267465	5.445594	-0.058406
6	1.358444	6.121594	2.298616
8	-0.199179	4.280776	1.528711
6	-1.634061	4.427654	1.104140
6	-1.801029	3.513000	-0.130536
6	-1.491672	4.187652	-1.464339
6	-2.222471	5.532483	-1.596626
6	-1.828735	6.488162	-0.460619
6	-2.111963	5.864868	0.917628
1	4.442390	-2.864801	-2.951091
1	3.378937	-1.466799	-3.200706
1	2.795698	-3.289584	-4.774848
1	3.566312	-5.217889	-3.376075
1	1.894258	-5.456948	-3.906452
1	2.706940	-4.183522	0.139653
1	4.046041	-4.476823	-0.990292
1	2.132930	-5.988298	-1.472041
1	-0.031119	-5.050953	-2.290033
1	0.296140	-4.526732	-0.625073
1	1.418421	-1.043646	-1.496924
1	1.175308	-2.206816	-0.161749
1	0.975175	-1.807747	-3.946863
1	0.361883	-3.446456	-4.242065
1	4.597871	-2.344186	-0.092294
1	5.037108	-0.226228	1.349615
1	6.825670	-0.169742	-1.037603
1	6.269695	1.987611	0.751369
1	5.316141	2.044576	-0.739235
1	3.061728	3.540981	-0.465425
1	2.449717	3.092499	3.665619
1	-0.218960	-0.495742	-2.030730
1	-3.109374	-2.525074	-0.626300
1	-3.293644	-1.352767	2.165076
1	0.900911	-2.845565	1.474076
1	0.250135	-3.875904	2.814652
1	0.038510	-4.371392	1.094775
1	-5.539820	-2.261193	1.074805
1	-4.834812	-3.872719	1.274091
1	-4.454192	-0.828428	3.460006
1	-5.292500	-0.743627	5.810331
1	-6.520648	-2.687105	6.761563
1	-6.911786	-4.708892	5.367650
1	-6.091530	-4.790440	3.027783
1	2.371389	6.522186	2.222989
1	0.648387	6.957154	2.287477
1	1.235571	5.555486	3.219180
1	-1.999535	0.801237	-1.833718
1	-3.979903	-1.462348	-2.515877
1	-3.072064	-0.598196	-3.754296
1	-0.409563	4.334992	-1.546698
1	-1.790498	3.490581	-2.263821
1	-1.987559	5.983134	-2.566122
1	-3.310863	5.364614	-1.588711
1	-0.769478	6.746344	-0.558508
1	-2.389616	7.425693	-0.537882
1	-1.742336	6.489214	1.739797
1	-3.200428	5.817035	1.060017
1	-2.143761	3.980498	1.963533
1	0.018911	3.371706	1.148280
1	-3.522249	1.792476	-4.248776
1	-2.869899	2.172202	-2.642253
1	-4.995741	3.324209	-2.012450
1	-4.328944	4.023869	-3.490316
1	-5.483976	0.122877	-4.460243
1	-6.184861	-0.583421	-2.997731
1	-7.617130	1.261901	-3.887232
1	-7.038809	1.623810	-2.257069
1	-5.892496	2.715454	-4.901158
1	-6.802592	3.626580	-3.690255
1	-4.704099	0.830682	-1.559606
6	9.896264	-1.056420	1.057084
1	10.685920	-1.219467	0.319059
1	10.132972	-0.198726	1.695151
1	9.749160	-1.950362	1.671837
6	4.692395	1.430188	3.346887
1	4.823860	0.405508	2.975282
1	5.677220	1.878302	3.509858
1	4.151151	1.399557	4.293752
1	-2.839534	3.154429	-0.136489
8	-0.896703	2.408458	0.057011
1	-1.392780	1.616929	0.381518

(1*S*,2*S*)$_{e,e}$-α
Et= -844.665013 (-2913.1337862)

6	-3.614977	1.481942	0.482702
6	-4.867692	0.600876	0.366261
6	-6.135443	1.459073	0.268030
6	-6.012606	2.438856	-0.910745
6	-4.771530	3.337655	-0.789996
6	-3.531235	2.462197	-0.679227
6	-1.545064	3.961019	-2.033183
8	-1.521978	3.155569	-2.871505
6	-1.696377	5.424886	-1.885100
7	0.359381	3.672676	-0.927883
6	1.364321	3.047469	-1.630299
6	2.580639	3.296469	-1.038971
7	2.291804	4.103417	0.059341
6	0.955247	4.302449	0.079400
6	3.972924	2.892792	-1.446562
6	4.528563	1.721600	-0.612265
7	5.996062	1.832506	-0.382144
6	6.441551	2.781211	0.578448
6	4.256643	0.344380	-1.260108
8	3.762556	0.226278	-2.372007
7	4.666523	-0.789017	-0.520426
6	4.117879	-2.174337	-0.728956
6	4.632913	-2.775270	-2.051085
6	4.097443	-4.200108	-2.210704
6	2.567401	-4.184176	-2.236051
6	2.037145	-3.596685	-0.917693
6	2.578826	-2.167521	-0.730516
6	4.582753	-5.068246	-1.050791
6	4.060810	-4.486033	0.261880
6	2.531407	-4.470180	0.246178
6	4.595712	-3.064345	0.442677
6	0.503960	-3.502620	-0.935468
8	-0.236200	-4.093393	-0.158793
7	-0.082913	-2.650580	-1.920973
6	-1.385211	-1.965942	-1.703582
6	-1.423750	-1.252226	-0.338219
7	-1.684776	-2.005160	0.812284
6	-1.586652	-1.416691	2.180075
6	-2.970226	-1.445289	2.851376
6	-2.994729	-0.591555	4.079289
6	-3.135766	0.793464	3.968646
6	-3.175292	1.585235	5.109705
6	-3.077840	1.001186	6.368679
6	-2.942807	-0.378103	6.483568
6	-2.901973	-1.174511	5.343852
6	-2.580885	-2.898314	-1.935975
8	-1.276020	-0.028725	-0.257572
8	5.748343	3.317533	1.437405
6	-0.541182	-2.216271	2.964324
8	0.717973	-1.698801	2.806178
6	1.817414	-2.417766	3.324739
8	-0.698918	-3.207620	3.640973
1	5.740697	-2.783804	-2.062829
1	4.317950	-2.159414	-2.916600
1	4.472053	-4.622620	-3.172856
1	5.689053	-5.114690	-1.040139
1	4.231646	-6.111098	-1.175232
1	4.244536	-2.659231	1.415803
1	5.702618	-3.082529	0.491328
1	4.408967	-5.116818	1.113712
1	2.136568	-5.500146	0.145375
1	2.143071	-4.085975	1.217209
1	2.194670	-1.518168	-1.548935
1	2.196057	-1.743271	0.220852
1	2.215835	-3.594952	-3.105848
1	2.175481	-5.210661	-2.376173
1	4.865909	-0.596797	0.438478
1	4.033518	1.726065	0.393642
1	6.539531	1.771036	-1.217443
1	4.641064	3.773595	-1.373607
1	3.943329	2.631501	-2.520754
1	1.156039	2.459710	-2.514198
1	0.464220	4.900360	0.834706
1	0.592800	-2.032791	-2.331256
1	-1.472215	-2.993953	0.725159
1	-1.258050	-0.344699	2.117372
1	2.654215	-1.741389	3.127392
1	1.725931	-2.614707	4.397803
1	1.958751	-3.361364	2.774241
1	-3.741205	-1.066507	2.135609
1	-3.267222	-2.485192	3.096592
1	-3.229804	1.259489	2.974242
1	-3.289609	2.670130	5.018026
1	-3.112120	1.626150	7.267384
1	-2.870631	-0.841211	7.473763
1	-2.795398	-2.262633	5.438631
1	-4.788838	-0.029314	-0.544646
1	-6.905793	3.071621	-0.988468
1	-5.932605	1.865615	-1.851855
1	-6.290405	2.011313	1.204847
1	-7.014376	0.821054	0.126323
1	-1.060494	5.908953	-2.630693
1	-2.752899	5.633364	-2.083789
1	-1.438076	5.753772	-0.882167
1	-1.453174	-1.166573	-2.498778
1	-2.658137	-3.675696	-1.148225
1	-2.429744	-3.457393	-2.882991
1	-4.897177	-0.086157	1.227021
6	-5.185876	-0.347820	-3.224355
6	-3.899656	-1.157017	-3.209219
6	-3.887295	-2.107653	-2.010788
6	-5.087162	-3.050760	-2.092337
6	-6.386569	-2.259779	-2.133224
6	-6.395663	-1.267727	-3.286524
1	-3.796955	-1.729903	-4.152624
1	-3.008874	-0.491088	-3.161887
1	-5.242520	0.294566	-2.307878
1	-5.189257	0.349789	-4.082948
1	-5.002093	-3.693371	-2.991642
1	-5.090161	-3.740386	-1.225629
1	-7.245636	-2.951989	-2.222306
1	-6.530528	-1.720265	-1.173969
1	-6.404863	-1.811408	-4.252209
1	-7.327417	-0.670358	-3.266152
1	-3.992811	-1.488390	-1.076347
1	-3.379782	1.927391	-1.625945
8	-2.352303	3.331745	-0.480025
1	-1.602134	2.779991	-0.172855
1	-2.700307	0.846548	0.477631
1	-3.627902	2.028139	1.441094
8	7.780758	2.977427	0.473127
6	8.418956	3.766175	1.460190
1	8.308398	3.331821	2.459056
1	9.462305	3.731940	1.135781
1	8.045044	4.795195	1.456069
6	3.245154	4.731122	0.970738
1	4.077307	4.039471	1.214028
1	3.660071	5.638622	0.522027
1	2.729765	4.996439	1.895311
1	-4.845160	3.953090	0.121013
8	-4.598355	4.173190	-1.935786
1	-5.437664	4.628985	-2.107871

(1*S*,2*S*)$_{e,e}$-β
Et=-844.666514 (-2913.1479319)

6	-2.755421	-3.418201	-1.814200
6	-1.692225	-2.374271	-1.436854
6	-2.061250	-1.555391	-0.188314
8	-2.085701	-0.316913	-0.222449
7	-0.330470	-2.962053	-1.329381
6	0.127884	-3.695639	-0.197557
8	-0.700285	-4.246100	0.518656
6	1.646870	-3.737009	0.029248
6	2.342608	-4.475733	-1.126435
6	3.856920	-4.456892	-0.908793
6	4.358528	-3.012480	-0.870494
6	3.677718	-2.256350	0.288171
6	2.152220	-2.282566	0.097664
6	4.196617	-5.155865	0.407157
6	3.508758	-4.421667	1.557590
6	4.007077	-2.976646	1.617482
6	1.994100	-4.444547	1.347863
7	4.153771	-0.833119	0.405832
6	4.076492	0.116899	-0.646668
8	3.350093	-0.049866	-1.614207
6	4.898276	1.406492	-0.441149
7	6.269048	1.109876	-0.945852
6	7.335971	1.923922	-0.451942
8	7.309341	2.598405	0.566446
6	4.273693	2.628464	-1.135883
6	3.075624	3.191992	-0.420979
6	1.778725	3.356470	-0.847547
7	1.038728	3.985586	0.129723
6	1.871109	4.213821	1.134314
7	3.113111	3.757095	0.851461
6	-0.917524	4.850570	-0.298064
6	-1.081664	5.642508	0.951999
8	-0.919230	5.109240	-1.443662
7	-2.406020	-2.199588	0.994950
6	-2.642493	-1.435274	2.254772
6	-1.883952	-2.112655	3.399732
8	-2.318399	-2.779565	4.311656
6	-4.154845	-1.326250	2.528296
6	-4.507640	0.023233	3.069180
6	-4.422454	1.148813	2.247115
6	-4.770232	2.402415	2.735515
6	-5.208900	2.542893	4.047649
6	-5.295142	1.424613	4.870543
6	-4.945746	0.167929	4.386138
8	-0.536169	-1.879858	3.317300
6	0.320985	-2.500259	4.253228
6	-2.553008	2.420165	-1.947915
6	-3.787341	1.734217	-2.525261
6	-4.990202	2.697802	-2.472679
6	-5.242774	3.248273	-1.056973
6	-3.983504	3.894824	-0.431275
6	-2.863930	2.874404	-0.519486
8	-1.575950	3.298727	0.098363
1	5.459538	-3.000172	-0.745774
1	4.148557	-2.518143	-1.839859
1	4.352570	-4.992183	-1.752862
1	5.292907	-5.176318	0.561716
1	3.870434	-6.213711	0.376720
1	3.533214	-2.452276	2.472613
1	5.098801	-2.968938	1.811247
1	3.750424	-4.930057	2.520785
1	1.624396	-5.488807	1.331128
1	1.480787	-3.950130	2.198571
1	1.866955	-1.749131	-0.836224
1	1.654508	-1.750174	0.933602
1	2.099741	-4.008164	-2.101019
1	1.977302	-5.519980	-1.182113
1	5.005793	-0.771203	0.923431
1	4.985419	1.628681	0.660611
1	6.289027	0.939758	-1.930200
1	5.037886	3.425949	-1.241749
1	3.955265	2.373258	-2.163602
1	1.336635	3.054696	-1.788218
1	1.626541	4.697242	2.069431
1	0.371725	-2.346629	-1.697082
1	-2.099803	-3.163605	1.073363
1	-2.229248	-0.395566	2.144658
1	1.310834	-2.208224	3.887191
1	0.153553	-2.117798	5.265217
1	0.217772	-3.591496	4.244551
1	-4.731927	-1.487051	1.593234
1	-4.493286	-2.124112	3.221385
1	-4.079154	1.046287	1.204388
1	-4.701477	3.278305	2.070760
1	-5.490915	3.529146	4.430682
1	-5.643093	1.531616	5.903932
1	-5.018307	-0.710470	5.039558
1	-3.135332	1.994846	0.095668
1	-5.577213	2.432645	-0.399524
1	-6.052167	3.984715	-1.075919
1	-5.885580	2.179785	-2.833387
1	-4.811171	3.532083	-3.163987
1	-4.009160	0.819704	-1.938293
1	-3.599052	1.395338	-3.555992
1	-0.938147	2.663836	-0.331062
1	-0.416766	6.507522	0.899753
1	-2.117816	5.997828	0.990067
1	-0.877151	5.040961	1.835090
1	-1.614126	-1.654823	-2.305198
1	-3.300731	-3.780636	-0.919578
1	-2.257013	-4.316885	-2.235023
6	-3.770273	-2.914247	-2.846985
6	-3.082240	-2.465816	-4.137466
1	-4.435271	-3.779808	-3.096208
6	-4.090975	-1.987646	-5.168065
1	-2.354735	-1.654170	-3.906927
1	-2.482075	-3.298901	-4.552476
6	-4.964523	-0.878051	-4.607764
1	-3.563641	-1.635856	-6.075619
1	-4.724807	-2.835948	-5.495993
6	-5.664369	-1.332390	-3.336145
1	-4.347287	0.027255	-4.395788
1	-5.710975	-0.563565	-5.361686
6	-4.656835	-1.797837	-2.295924
1	-6.271278	-0.502033	-2.923199
1	-6.378548	-2.147657	-3.566221
1	-4.037932	-0.927527	-1.973538
1	-5.181502	-2.148054	-1.385443
8	8.435630	1.792192	-1.240660
6	9.636574	2.406638	-0.812832
1	10.329966	2.127460	-1.610395
1	9.532548	3.494928	-0.752849
1	9.973078	2.009644	0.150410
6	4.283118	3.889197	1.718010
1	4.779710	2.916530	1.829327
1	4.995223	4.605529	1.297228
1	3.960210	4.238889	2.699605
1	-4.183045	4.147818	0.623001
1	-2.289591	3.290073	-2.554798
1	-3.718614	4.811410	-0.971605
8	-1.356486	1.631055	-1.902146
1	-1.585760	0.736146	-1.549114

(1*S*,2*S*)$_{a,a}$-β

Et=-844.644630(-2913.1427901)

6	-6.030156	1.918283	-4.641293
6	-4.803990	2.421988	-3.895885
6	-3.794774	1.303197	-3.700914
6	-4.423174	0.126799	-2.950936
6	-5.641024	-0.385015	-3.719475
6	-6.654415	0.730504	-3.925510
6	-3.406116	-0.999206	-2.750352
6	-2.289005	-0.562696	-1.791945
6	-2.718522	-0.618055	-0.312463
8	-2.670662	0.390056	0.402702
7	-1.016248	-1.287804	-2.046086
6	-0.784717	-2.651464	-1.725272
8	-1.747513	-3.367214	-1.471985
6	0.669133	-3.148983	-1.772901
6	1.128947	-3.212047	-3.239637
6	2.576837	-3.699411	-3.305438
6	3.483022	-2.727923	-2.548228
6	3.043809	-2.652985	-1.072569
6	1.578583	-2.187759	-0.983875
6	2.679744	-5.093040	-2.686683
6	2.233689	-5.029119	-1.226327
6	0.783910	-4.551017	-1.151306
6	3.138266	-4.068449	-0.453914
7	3.914862	-1.738440	-0.253106
6	4.200218	-0.394248	-0.596920
8	3.513399	0.223050	-1.397545
6	5.349281	0.263146	0.196531
7	6.621139	-0.350915	-0.279240
6	7.738490	-0.304032	0.614445
8	7.681628	-0.113875	1.819586
6	5.368786	1.795058	0.069790
6	4.242653	2.472974	0.800049
6	3.213435	3.244515	0.321246
7	2.434642	3.695069	1.364407
6	2.988174	3.212509	2.471491
7	4.080775	2.469057	2.184063
7	-3.206986	-1.814837	0.212157
6	-3.352087	-2.043203	1.677011
6	-2.227467	-2.966661	2.158227
8	-2.296443	-4.071438	2.645738
6	-4.741697	-2.631603	1.967357
6	-5.179552	-2.395238	3.378284
6	-4.979925	-1.154822	3.987940
6	-5.435272	-0.925709	5.279616
6	-6.091926	-1.936287	5.975174
6	-6.286070	-3.176217	5.376342
6	-5.831651	-3.408336	4.082239
8	8.890290	-0.572603	-0.055534
8	-0.986926	-2.404718	1.974076
6	0.157175	-3.206154	2.173217
6	1.055493	5.359981	0.815901
8	1.214104	5.467214	-0.333065
6	1.185604	6.212089	2.022892
8	-0.226580	4.180117	1.304258
6	-1.663248	4.020157	0.877273
6	-1.813877	3.404532	-0.531823
6	-1.643896	4.412182	-1.672140
6	-2.507429	5.666177	-1.466772
6	-2.205620	6.333299	-0.116331
6	-2.399382	5.343973	1.045938
8	-3.138534	2.896290	-0.596594
1	4.537064	-3.061973	-2.620754
1	3.437882	-1.729328	-3.026282
1	2.899290	-3.741756	-4.372612
1	3.718073	-5.471175	-2.757664
1	2.051496	-5.811069	-3.248906
1	2.837333	-4.047027	0.613768
1	4.182106	-4.441833	-0.478183
1	2.306437	-6.044602	-0.769988
1	0.118704	-5.262125	-1.679597
1	0.437551	-4.532686	-0.091818
1	1.469969	-1.155511	-1.382695
1	1.258456	-2.152525	0.084713
1	1.043105	-2.216821	-3.718799
1	0.470723	-3.893548	-3.813622
1	4.698364	-2.218840	0.138300
1	5.228934	-0.001890	1.286336
1	6.830857	-0.115457	-1.227143
1	6.336729	2.187951	0.442983
1	5.302011	2.097513	-0.991315
1	2.988155	3.499453	-0.705667
1	2.635797	3.370453	3.481461
1	-0.202480	-0.712065	-1.940263
1	-3.010786	-2.640047	-0.343889
1	-3.268156	-1.062504	2.229411
1	0.958416	-2.562412	1.782588
1	0.312095	-3.436015	3.231138
1	0.122168	-4.135476	1.580940
1	-5.496556	-2.163987	1.300806
1	-4.762963	-3.716013	1.732637
1	-4.445906	-0.369667	3.432317
1	-5.278815	0.050667	5.749125
1	-6.453758	-1.755714	6.992757
1	-6.798143	-3.974487	5.924301
1	-5.983924	-4.389866	3.617847
1	2.145388	6.731668	1.965889
1	0.374956	6.949768	1.992218
1	1.109924	5.628488	2.936463
1	-2.057449	0.516688	-2.040031
1	-3.921595	-1.912117	-2.388680
1	-2.971714	-1.280888	-3.732463
1	-0.587901	4.690825	-1.756100
1	-1.921869	3.898735	-2.599759
1	-2.332927	6.373766	-2.284178
1	-3.566533	5.384804	-1.508069
1	-1.181501	6.730354	-0.127368
1	-2.864520	7.193933	0.041637
1	-2.143876	5.785451	2.016681
1	-3.460825	5.074043	1.099265
1	-2.027674	3.295242	1.613950
1	-1.080188	2.587735	-0.649879
1	0.269420	3.346135	1.186593
1	-3.156116	1.989728	-0.214355
1	-3.406201	0.964778	-4.682384
1	-2.909997	1.670019	-3.131168
1	-5.098744	2.839733	-2.911911
1	-4.335970	3.258262	-4.450164
1	-5.323010	-0.797360	-4.698207
1	-6.110283	-1.226594	-3.173288
1	-7.518146	0.350715	-4.504415
1	-7.063990	1.052827	-2.947231
1	-5.751005	1.631254	-5.674780
1	-6.772840	2.732554	-4.743419
1	-4.763634	0.488191	-1.947637
6	10.078027	-0.721699	0.699918
1	10.813959	-0.941997	-0.077731
1	10.336828	0.201485	1.228617
1	10.003835	-1.551404	1.410384
6	4.950473	1.811517	3.159435
1	5.117373	0.767505	2.863800
1	5.915388	2.323426	3.220273
1	4.469280	1.833673	4.138269

Catalyst Boc-(π-Me)His-^{A}Gly-Cha-Phe-OMe

(1*R*,2*R*)$_{e,e}$-α			
Et=-844.689656 (-3031. 1076024)			
6	-2.320286	3.274796	-0.550651
6	-3.674983	2.951574	-1.188659
6	-4.658977	4.117703	-0.967265
6	-4.093000	5.460352	-1.458769
6	-2.717341	5.766696	-0.830446
6	-1.793390	4.593362	-1.099190
6	0.724359	5.569133	-1.445889
8	0.590268	5.365425	-2.590370
6	1.202090	6.702230	-0.611246
7	2.165835	4.028181	-0.703526
6	2.381842	2.835531	-1.361203
6	3.654177	2.378757	-1.108180
7	4.227144	3.340470	-0.279430
6	3.300185	4.300172	-0.069360
6	4.374400	1.152357	-1.601714
6	4.547434	0.077648	-0.510900
7	5.826854	-0.676132	-0.640241
6	7.020928	-0.044882	-0.177607
6	3.429484	-0.989112	-0.535353
8	2.805178	-1.265397	-1.547986
7	3.124712	-1.581163	0.716331
6	2.344087	-2.857487	0.878138
6	2.959057	-4.028874	0.085602
6	2.144084	-5.299810	0.330292
6	0.701924	-5.087608	-0.133597
6	0.070670	-3.930497	0.658538
6	0.886417	-2.643379	0.436068
6	2.160189	-5.645523	1.819039
6	1.536589	-4.494990	2.609176
6	0.092776	-4.284695	2.154107
6	2.347477	-3.218885	2.382889
6	-1.367639	-3.683337	0.178751
8	-2.359902	-3.868206	0.864204
7	-1.540350	-3.232003	-1.171261
6	-2.727086	-2.427041	-1.574096
6	-2.810293	-1.165714	-0.694150
7	-3.870021	-0.997998	0.213490
6	-3.755748	-0.095907	1.395581
6	-5.027896	0.760200	1.490371
6	-5.012101	1.672265	2.674699
6	-4.184779	2.796582	2.690367
6	-4.189357	3.655172	3.782610
6	-5.022819	3.400040	4.866908
6	-5.851501	2.283274	4.855143
6	-5.848408	1.420853	3.763745
6	-4.007059	-3.270516	-1.624820
8	-1.963814	-0.276865	-0.800331
8	7.053553	0.922085	0.577328
6	-3.535833	-0.955367	2.647171
8	-2.279123	-0.796387	3.159243
6	-1.833749	-1.664989	4.180247
8	-4.320480	-1.720811	3.163228
1	4.011681	-4.192448	0.390593
1	2.979360	-3.801776	-0.998884
1	2.594517	-6.138788	-0.250867
1	3.196688	-5.832338	2.160880
1	1.601824	-6.584165	2.001970
1	1.920273	-2.390893	2.983331
1	3.383011	-3.369356	2.750389
1	1.543927	-4.743457	3.696693
1	-0.502673	-5.201063	2.337844
1	-0.395099	-3.481915	2.754214
1	0.837871	-2.358312	-0.638740
1	0.433371	-1.806144	1.004223
1	0.685098	-4.877452	-1.221271
1	0.112522	-6.013752	0.013986
1	3.878979	-1.524728	1.368696
1	4.552817	0.577363	0.492804
1	5.906035	-1.166747	-1.507299
1	5.360027	1.449965	-2.012207
1	3.803574	0.754710	-2.461514
1	1.611319	2.372075	-1.963333
1	3.495865	5.170671	0.540417
1	-0.690818	-2.847059	-1.542800
1	-4.421075	-1.824557	0.366848
1	-2.884265	0.598379	1.257187
1	-0.952939	-1.144234	4.565221
1	-2.566735	-1.815108	4.979971
1	-1.540386	-2.632394	3.743219
1	-5.105587	1.372760	0.559323
1	-5.932277	0.118248	1.515437
1	-3.527818	3.004318	1.831929
1	-3.537185	4.534325	3.789286
1	-5.026978	4.077754	5.727240
1	-6.509480	2.080022	5.707269
1	-6.501670	0.539306	3.762171
1	-3.531993	2.754261	-2.258690
1	-4.786990	6.273571	-1.223633
1	-3.993533	5.440047	-2.552382
1	-4.892867	4.188724	0.105281
1	-5.603478	3.899823	-1.476019
1	2.145140	7.066291	-1.025103
1	0.453154	7.499932	-0.682176
1	1.312103	6.410789	0.431170
1	-2.518336	-2.088939	-2.631397
1	-4.478619	-3.348049	-0.618730
1	-3.758121	-4.313968	-1.909772
1	-4.083916	2.033355	-0.730450
6	-5.483348	-2.213499	-5.043308
6	-4.479598	-2.783133	-4.055062
6	-5.014956	-2.699043	-2.624784
6	-6.343378	-3.449058	-2.524869
6	-7.353241	-2.890867	-3.515868
6	-6.815545	-2.939773	-4.937562
1	-4.250159	-3.836927	-4.312099
1	-3.510718	-2.238946	-4.116404
1	-5.626251	-1.130263	-4.857601
1	-5.086374	-2.293994	-6.073387
1	-6.180920	-4.529348	-2.714002
1	-6.744253	-3.378562	-1.494667
1	-8.299575	-3.461294	-3.448950
1	-7.609901	-1.847009	-3.245445
1	-6.695704	-3.993757	-5.258793
1	-7.548261	-2.492098	-5.636009
1	-5.199285	-1.623399	-2.378517
1	-1.590420	4.473347	-2.168566
8	-0.473696	4.792175	-0.447849
1	-0.098126	3.881118	-0.336036
1	-2.300907	6.688348	-1.253517
8	8.083696	-0.720027	-0.658465
6	9.443837	-0.444640	-0.215957
6	5.613103	3.414184	0.174877
1	6.000022	2.412521	0.453727
1	6.249328	3.829424	-0.612608
1	5.664349	4.062655	1.051151
1	-2.814897	5.914351	0.252373
1	-2.461515	3.373159	0.543946
8	-1.265017	2.355624	-0.820842
1	-1.536315	1.436494	-0.597160
6	9.890502	0.960936	-0.617073
1	10.969263	1.075300	-0.445483
1	9.703300	1.159060	-1.680604
1	9.383765	1.741543	-0.034462
6	9.607026	-0.668424	1.286647
1	10.670398	-0.631878	1.558757
1	9.092009	0.097928	1.880968
1	9.221166	-1.648959	1.595325
6	10.255695	-1.491229	-0.991550
1	11.322745	-1.396505	-0.750249
1	9.949790	-2.515596	-0.739947
1	10.150510	-1.369390	-2.077923

($1R,2R$)$_{e,e}$-β
Et=-844.678784(-3031.0892541)

6	–3.721394	–2.543913	–2.077184
6	–2.569749	–1.641167	–1.598890
6	–2.795009	–1.036303	–0.198118
8	–2.657020	0.171407	0.003992
7	–1.253619	–2.335109	–1.671852
6	–0.870442	–3.381555	–0.786144
8	–1.743448	–3.962794	–0.151472
6	0.625781	–3.719332	–0.707582
6	1.110694	–4.288562	–2.051364
6	2.609318	–4.586332	–1.971901
6	3.381141	–3.299818	–1.671620
6	2.911816	–2.718925	–0.323626
6	1.401458	–2.429443	–0.382447
6	2.869387	–5.614809	–0.871732
6	2.394226	–5.050433	0.466534
6	3.163017	–3.768191	0.786068
6	0.896797	–4.751014	0.399445
7	3.644121	–1.466370	0.069826
6	3.703178	–0.289294	–0.720883
8	3.017141	–0.139404	–1.719992
6	4.611494	0.820984	–0.154454
7	5.989876	0.548465	–0.645793
6	7.074788	1.110042	0.107874
8	6.991291	1.483054	1.268467
6	4.125934	2.230104	–0.527503
6	2.814281	2.609212	0.104338
6	1.629034	2.983761	–0.478864
7	0.702013	3.302351	0.489402
6	1.318006	3.135968	1.652622
7	2.593065	2.719321	1.476076
6	–0.889746	4.698965	–0.123953
6	–1.058156	5.459287	1.138425
8	–0.646254	4.937105	–1.242437
7	–3.188451	–1.887024	0.843390
6	–3.166643	–1.456923	2.269311
6	–2.075180	–2.243935	3.003248
8	–2.181036	–3.253967	3.661295
6	–4.549390	–1.688636	2.897945
6	–4.762720	–0.864393	4.127993
6	–4.369121	0.474888	4.165778
6	–4.615930	1.248387	5.292311
6	–5.257182	0.689202	6.393271
6	–5.644584	–0.646150	6.364655
6	–5.398585	–1.423299	5.237437
8	–0.831901	–1.688128	2.832002
6	0.292352	–2.395231	3.313081
6	–2.903296	2.689691	–2.178208
6	–4.203572	2.541315	–2.988099
6	–4.984199	3.860541	–3.060320
6	–5.245838	4.436428	–1.659236
6	–3.946689	4.590053	–0.856657
6	–3.237965	3.231774	–0.789173
8	–2.044449	3.350168	0.092893
1	4.468575	–3.510601	–1.643889
1	3.225320	–2.571219	–2.491782
1	2.951651	–4.995331	–2.951741
1	3.946893	–5.865624	–0.824631
1	2.342328	–6.562158	–1.097697
1	2.841438	–3.374788	1.772884
1	4.244351	–3.996223	0.876371
1	2.580318	–5.798440	1.273104
1	0.326391	–5.680692	0.206794
1	0.538918	–4.365980	1.381929
1	1.179817	–1.659049	–1.153991
1	1.054386	–2.016633	0.588176
1	0.912562	–3.575486	–2.875776
1	0.550119	–5.212174	–2.295513
1	4.504635	–1.663731	0.537283
1	4.632754	0.742273	0.970497
1	6.067322	0.640814	–1.637913
1	4.898696	2.973798	–0.243231
1	3.999550	2.320156	–1.622108
1	1.394546	3.052662	–1.532479
1	0.887580	3.298278	2.631001
1	–0.494968	–1.719868	–1.899522
1	–2.999278	–2.870088	0.674931
1	–2.938249	–0.354091	2.336646
1	1.117781	–1.718678	3.073620
1	0.242721	–2.575100	4.391964
1	0.420592	–3.349255	2.775478
1	–5.343668	–1.418589	2.170917
1	–4.701556	–2.765125	3.122042
1	–3.847632	0.898188	3.294672
1	–4.306299	2.297903	5.313946
1	–5.454552	1.298856	7.281266
1	–6.144919	–1.089541	7.232486
1	–5.703068	–2.476781	5.223087
1	–3.871323	2.518419	–0.244278
1	–5.927419	3.771316	–1.106486
1	–5.731167	5.415960	–1.716115
1	–5.934467	3.707399	–3.582308
1	–4.415731	4.590523	–3.652211
1	–4.827593	1.756184	–2.521756
1	–3.971918	2.169834	–3.998813
1	–1.490108	2.545207	0.030518
1	–0.268622	6.212536	1.190177
1	–2.045547	5.933238	1.095099
1	–1.032499	4.801662	2.004061
1	–2.477370	–0.787333	–2.332321
1	–4.453160	–2.719031	–1.262356
1	–3.331290	–3.550799	–2.336340
6	–4.482265	–2.007919	–3.293488
6	–3.546495	–1.609199	–4.433913
1	–5.131531	–2.843889	–3.659455
6	–4.329648	–1.132181	–5.645693
1	–2.856379	–0.809135	–4.080288
1	–2.901793	–2.465823	–4.710087
6	–5.255367	0.016897	–5.282989
1	–3.631968	–0.820724	–6.446744
1	–4.918539	–1.971511	–6.067098
6	–6.186084	–0.371563	–4.144533
1	–4.655833	0.910616	–4.991305
1	–5.844496	0.324984	–6.167609
6	-5.401938	-0.843097	-2.928717
1	-6.823915	0.490404	-3.867041
1	-6.880342	-1.167869	-4.479275
1	-4.813756	0.007365	-2.512087
1	-6.098789	-1.148705	-2.123997
8	8.183860	1.096912	-0.662014
6	9.498134	1.423035	-0.127484
6	3.569937	2.497658	2.541767
1	4.046855	1.517327	2.417504
1	4.341112	3.273542	2.521220
1	3.057456	2.525269	3.504414
1	-2.404707	1.712539	-2.090330
1	-2.211260	3.372824	-2.683326
1	-3.295643	5.300646	-1.377903
8	-4.148823	5.162227	0.429686
1	-4.866510	4.683436	0.876324
6	9.573414	2.879937	0.328673
1	10.615224	3.153096	0.543600
1	9.205222	3.567370	-0.444098
1	8.994174	3.060412	1.243834
6	9.904718	0.471654	0.997080
1	9.785865	-0.579374	0.702584
1	10.961068	0.624560	1.255564
1	9.318840	0.633088	1.911688
6	10.407546	1.210337	-1.345694
1	11.451184	1.425494	-1.080578
1	10.366247	0.175789	-1.711930
1	10.135870	1.870389	-2.180283

$(1R,2R)_{a,a}$-β

Et=-844.670899 (-3031.0921356)

6	3.660074	2.336737	-1.149002
6	2.402486	1.455439	-1.090296
6	2.197942	0.749265	0.263411
8	2.030158	-0.478250	0.344464
7	1.186497	2.215557	-1.491583
6	0.612049	3.262727	-0.712306
8	1.271285	3.748168	0.199490
6	-0.811125	3.700256	-1.089005
6	-0.860994	4.187565	-2.547611
6	-2.298472	4.559410	-2.916175
6	-3.206760	3.336174	-2.770750
6	-3.177927	2.843581	-1.312006
6	-1.733651	2.481967	-0.914263
6	-2.786317	5.682775	-2.002570
6	-2.743959	5.202546	-0.552549
6	-1.309616	4.829698	-0.173016
6	-3.660061	3.988991	-0.390307
7	-4.095944	1.668164	-1.121103
6	-3.783264	0.359605	-1.569750
8	-3.128260	0.187313	-2.586180
6	-4.363195	-0.805513	-0.740846
7	-5.843752	-0.775167	-0.889018
6	-6.618351	-1.424656	0.125719
8	-6.208726	-1.682931	1.248886
6	-3.769615	-2.167918	-1.133281
6	-2.348867	-2.372254	-0.680961
6	-1.216684	-2.619485	-1.416344
7	-0.149814	-2.844397	-0.576077
6	-0.620127	-2.742749	0.660056
7	-1.942629	-2.454576	0.650827
6	1.447096	-3.874139	-1.528239
8	2.584304	-2.751082	-0.899195
6	3.888256	-2.369014	-1.532686
6	3.758315	-1.518979	-2.801556
6	3.658136	-2.287344	-4.128689
6	4.707738	-3.404407	-4.216819
6	4.590219	-4.357044	-3.019175
6	4.771576	-3.623551	-1.682284
7	2.211678	1.509238	1.421949
6	1.900780	0.954494	2.767944
6	0.661454	1.660460	3.325721
8	0.549554	2.340101	4.318874
6	3.125506	1.113919	3.683441
6	3.131732	0.125855	4.806613
6	2.798885	-1.211551	4.581482
6	2.856052	-2.133991	5.617817
6	3.243437	-1.726687	6.890743
6	3.567548	-0.394409	7.123086
6	3.512029	0.531671	6.086405
8	-0.442112	1.444775	2.535869
6	-1.622151	2.176790	2.792251
6	1.540862	-5.042496	-0.603972
8	1.221976	-3.776409	-2.679732
1	-4.242364	3.595268	-3.067223
1	-2.876432	2.538502	-3.465288
1	-2.323586	4.905833	-3.976352
1	-3.815021	5.985329	-2.279096
1	-2.155757	6.584433	-2.127885
1	-3.663740	3.666674	0.672135
1	-4.703787	4.270383	-0.634902
1	-3.097171	6.018815	0.120954
1	-0.647212	5.713224	-0.259569
1	-1.263570	4.512253	0.889095
1	-1.353706	1.640296	-1.534688
1	-1.710389	2.138544	0.147014
1	-0.490466	3.408362	-3.242419
1	-0.193854	5.062512	-2.675353
1	-4.549920	1.686748	-0.231983
1	-4.128397	-0.620284	0.346649
1	-6.141711	-0.932985	-1.829427
1	-4.399771	-2.981483	-0.718658
1	-3.785661	-2.296493	-2.231024
1	-1.105892	-2.663577	-2.490915
1	-0.045508	-2.845126	1.570599
1	0.492760	1.642047	-1.934139
1	2.113921	2.512015	1.296959
1	1.670198	-0.147495	2.686411
1	-2.171644	2.056659	1.846801
1	-2.175046	1.739448	3.628672
1	-1.437299	3.241626	2.979828
1	4.056603	0.961956	3.095162
1	3.184675	2.148933	4.079321
1	2.479465	-1.516705	3.574189
1	2.598102	-3.181569	5.433112
1	3.290976	-2.453757	7.708389
1	3.867129	-0.070852	8.125982
1	3.764152	1.581587	6.278122
1	0.652753	-5.660719	-0.749410
1	2.426340	-5.624327	-0.882971
1	1.627691	-4.733175	0.435286
1	2.509410	0.652025	-1.876188
1	3.737453	3.004195	-0.265775
1	3.558312	3.023089	-2.017554
1	2.656927	-2.715094	-4.239627
1	3.790890	-1.576639	-4.951577
1	4.582427	-3.964672	-5.149189
1	5.714467	-2.970270	-4.237295
1	3.613468	-4.857186	-3.040878
1	5.340096	-5.157606	-3.077786
1	4.339473	-1.766930	-0.735649
1	2.914457	-0.816586	-2.684202
1	2.084034	-1.926183	-0.636853
1	4.663507	-0.887455	-2.806485
6	7.321406	1.648412	-2.160345
6	6.021231	2.415188	-1.978416
6	4.958782	1.540178	-1.306840
6	5.488003	1.036349	0.037035
6	6.789206	0.270052	-0.141354
6	7.838809	1.127037	-0.829632
1	6.196730	3.325096	-1.369942
1	5.655497	2.772603	-2.961365
1	7.166593	0.804460	-2.862753
1	8.079650	2.301103	-2.634019
1	5.642257	1.889523	0.728685
1	4.735363	0.383576	0.524005
1	7.162683	-0.070665	0.843359
1	6.603922	-0.651526	-0.731515
1	8.122095	1.975776	-0.175548
1	8.765281	0.541513	-0.984165
1	4.778329	0.650024	-1.971717
8	-7.861579	-1.641936	-0.353302
6	-8.948231	-2.102394	0.498696
6	-2.791536	-2.299869	1.832134
1	-3.383496	-1.379878	1.745808
1	-3.470913	-3.151680	1.931381
1	-2.159624	-2.237062	2.719117
6	-10.135651	-2.130095	-0.473751
1	-11.042449	-2.466486	0.046142
1	-10.344492	-1.136878	-0.893376
1	-9.962085	-2.816603	-1.313165
6	-8.683717	-3.508936	1.035426
1	-9.590999	-3.907216	1.509109
1	-8.398697	-4.202864	0.233839
1	-7.888211	-3.523212	1.792054
6	-9.230982	-1.122355	1.636494
1	-9.352339	-0.095558	1.266996
1	-10.161011	-1.400448	2.150065
1	-8.431880	-1.116656	2.389582
1	4.555383	-4.299995	-0.839442
8	6.085174	-3.087337	-1.554360
1	6.724013	-3.785386	-1.768993

(1R,2S)e,a-α

Et=-844.688829(-3031.1124904)

6	3.321362	-2.924787	-0.552755
6	4.686278	-2.863519	0.141285
6	4.882570	-3.967425	1.188750
6	4.604294	-5.353436	0.594484
6	3.168458	-5.428754	0.047221
6	2.931479	-4.346879	-1.001971
6	0.944514	-3.868614	-2.774581
8	1.370562	-2.856562	-3.198828
6	0.510177	-5.142972	-3.416939
7	-0.999009	-3.355853	-1.823093
6	-1.682454	-2.264644	-2.304699
6	-2.969650	-2.260547	-1.817870
7	-3.057237	-3.394930	-1.015741
6	-1.855840	-4.016005	-1.054987
6	-4.119722	-1.323662	-2.077165
6	-4.332323	-0.305549	-0.938655
7	-5.772581	-0.012126	-0.697848
6	-6.539517	-0.978841	0.015843
6	-3.624582	1.042688	-1.204921
8	-3.088609	1.310340	-2.271215
7	-3.681524	1.992094	-0.161783
6	-2.807304	3.211540	-0.065944
6	-3.199255	4.245178	-1.140085
6	-2.335710	5.498948	-0.987284
6	-0.858917	5.138986	-1.161720
6	-0.448237	4.116593	-0.088847
6	-1.317784	2.851718	-0.215681
6	-2.555812	6.113469	0.394215
6	-2.152106	5.099160	1.463195
6	-0.675312	4.737964	1.298392
6	-3.012965	3.841742	1.331972
6	1.016613	3.695264	-0.276024
8	1.906624	3.895005	0.542456
7	1.347892	3.020431	-1.487255
6	2.524265	2.118160	-1.607713
6	2.522125	1.057501	-0.490129
7	2.963709	1.409459	0.788294
6	2.725455	0.534393	1.975702
6	4.074677	0.073294	2.550998
6	3.912108	-0.705598	3.817321
6	3.484472	-2.033719	3.780470
6	3.346311	-2.757393	4.958798
6	3.641573	-2.164159	6.181855
6	4.079661	-0.844892	6.222795
6	4.216122	-0.116255	5.046007
6	3.843541	2.893951	-1.712852
8	2.154050	-0.099420	-0.721650
8	-6.065426	-1.877784	0.704797
6	1.893968	1.338001	2.981660
8	0.561165	1.029224	2.901741
6	-0.354333	1.784478	3.667778
8	2.265710	2.189713	3.757051
1	-4.270756	4.510233	-1.044746
1	-3.072211	3.826366	-2.158021
1	-2.624832	6.236944	-1.772368
1	-3.615809	6.407451	0.521203
1	-1.963043	7.042519	0.502801
1	-2.739632	3.122335	2.133272
1	-4.079212	4.098513	1.490694
1	-2.307275	5.542736	2.475063
1	-0.042312	5.638476	1.422483
1	-0.362906	4.030164	2.099617
1	-1.129961	2.372736	-1.202685
1	-1.022008	2.114179	0.558719
1	-0.691007	4.736215	-2.180040
1	-0.230352	6.047158	-1.077816
1	-3.927264	1.614470	0.728539
1	-3.914376	-0.731163	0.010388
1	-6.225374	0.416641	-1.478177
1	-5.040096	-1.916965	-2.245115
1	-3.921883	-0.807903	-3.035365
1	-1.212257	-1.548962	-2.966053
1	-1.650540	-4.930153	-0.515477
1	0.539104	2.656820	-1.956470
1	2.969568	2.410599	0.965751
1	2.152105	-0.385980	1.669016
1	-1.308538	1.303652	3.435219
1	-0.145157	1.729225	4.740938
1	-0.370695	2.835496	3.337533
1	4.584567	-0.567951	1.790297
1	4.744298	0.940776	2.722112
1	3.276717	-2.519297	2.813549
1	3.009362	-3.798522	4.921985
1	3.533493	-2.736026	7.109615
1	4.318584	-0.376017	7.183642
1	4.555762	0.926441	5.085055
1	5.462495	-2.937148	-0.632507
1	4.739155	-6.133176	1.350962
1	5.324646	-5.568457	-0.207421
1	4.202558	-3.781308	2.037651
1	5.902397	-3.918197	1.584038
1	-0.120727	-4.897108	-4.273359
1	1.406305	-5.660413	-3.781620
1	-0.023002	-5.785736	-2.720847
1	2.395307	1.578258	-2.592226
1	4.171863	3.290123	-0.730004
1	3.693905	3.790738	-2.350324
1	4.791569	-1.865098	0.602427
6	5.726972	0.798157	-4.363602
6	4.635269	1.673673	-3.772083
6	4.946029	2.020558	-2.314897
6	6.296605	2.731234	-2.230038
6	7.397153	1.867872	-2.827714
6	7.080372	1.485525	-4.265208
1	4.530832	2.602627	-4.368417
1	3.645361	1.167880	-3.825629
1	5.757582	-0.177125	-3.838032
1	5.493888	0.565219	-5.420244
1	6.244333	3.703524	-2.760183
1	6.534971	2.973034	-1.175743
1	8.362941	2.407109	-2.783630
1	7.533527	0.953837	-2.215663
1	7.089507	2.389875	-4.905945
1	7.872242	0.823634	-4.665181
1	5.011204	1.069413	-1.729125
1	3.397400	-4.592947	-1.958668
8	1.455416	-4.289957	-1.242697
1	1.198678	-3.519012	-0.636368
1	2.953132	-6.410878	-0.386819
8	-7.849109	-0.704228	-0.149283
6	-8.887164	-1.389229	0.608267
6	-4.241358	-3.901471	-0.329164
1	-4.794153	-3.078937	0.170091
1	-4.910315	-4.399478	-1.037398
1	-3.928687	-4.622496	0.427860
1	2.461951	-5.273355	0.871591
1	3.314893	-2.268213	-1.431195
8	2.234434	-2.546277	0.322578
1	2.122913	-1.561311	0.285558
6	-8.942857	-2.877455	0.264143
1	-8.078735	-3.428962	0.657552
1	-9.843800	-3.330068	0.699637
1	-8.982567	-3.042609	-0.820544
6	-10.162792	-0.691959	0.115615
1	-11.043384	-1.119164	0.613437
1	-10.150594	0.384680	0.332249
1	-10.304228	-0.812380	-0.966792
6	-8.725685	-1.175935	2.112610
1	-7.858191	-1.712486	2.519176
1	-8.610494	-0.112770	2.361685
1	-9.614488	-1.544386	2.642131

$(1R,2S)_{e,a}$-β

Et= -844.684437 (-3031.086819)

6	3.440549	3.415987	-1.500331
6	2.316144	2.381651	-1.336606
6	2.503420	1.415253	-0.151735
8	2.365094	0.199767	-0.292409
7	0.975862	3.029887	-1.267084
6	0.529641	3.758263	-0.126492
8	1.364603	4.182032	0.664792
6	-0.985692	3.957374	0.024720
6	-1.548352	4.763549	-1.157880
6	-3.065407	4.899103	-1.010739
6	-3.714583	3.513508	-1.000224
6	-3.166363	2.694772	0.184901
6	-1.638892	2.563020	0.058890
6	-3.390219	5.632716	0.289965
6	-2.835558	4.833700	1.468579
6	-3.481924	3.448307	1.499485
6	-1.319233	4.695358	1.330892
7	-3.778857	1.325765	0.292403
6	-3.750330	0.352363	-0.739912
8	-3.057681	0.481413	-1.737319
6	-4.575212	-0.919308	-0.454049
7	-5.976922	-0.621743	-0.859528
6	-7.013249	-1.418962	-0.268723
8	-6.889366	-2.065090	0.761179
6	-4.015000	-2.162423	-1.162901
6	-2.711649	-2.655462	-0.595250
6	-1.487586	-2.816513	-1.197615
7	-0.590055	-3.371914	-0.312290
6	-1.259949	-3.555852	0.817607
7	-2.543172	-3.141537	0.699904
6	1.171702	-4.394588	-1.249742
6	1.232835	-5.606114	-0.404508
8	1.080607	-4.100650	-2.369798
7	2.850292	1.939849	1.103489
6	2.821789	1.096174	2.331981
6	1.835074	1.710131	3.330184
8	2.056087	2.451848	4.260825
6	4.242240	0.976956	2.916438
6	4.479303	-0.394502	3.463880
6	4.557075	-1.483988	2.594265
6	4.781772	-2.762692	3.088476
6	4.941727	-2.963797	4.455187
6	4.872371	-1.880436	5.325198
6	4.639816	-0.599186	4.834660
8	0.544024	1.330318	3.066192
6	-0.506896	1.958448	3.770118
6	3.598089	-2.242450	-2.106780
6	5.008989	-1.690082	-2.372493
6	6.086906	-2.742967	-2.080006
6	5.957797	-3.293628	-0.651010
6	4.545404	-3.824284	-0.346097
6	3.530637	-2.728031	-0.661784
8	2.183461	-3.196832	-0.247798
1	-4.815413	3.613997	-0.924347
1	-3.513500	2.999918	-1.961295
1	-3.464303	5.480719	-1.875143
1	-4.484316	5.767284	0.394723
1	-2.954682	6.650783	0.277139
1	-3.104958	2.878549	2.374363
1	-4.576631	3.552760	1.641466
1	-3.067630	5.365955	2.421209
1	-0.838635	5.693182	1.341008
1	-0.903953	4.143997	2.205692
1	-1.366514	2.007423	-0.865901
1	-1.235397	1.979150	0.912564
1	-1.309593	4.273900	-2.122553
1	-1.076444	5.765088	-1.191430
1	-4.643779	1.338331	0.791876
1	-4.579236	-1.116749	0.656174
1	-6.065756	-0.469551	-1.843312
1	-4.763130	-2.980730	-1.119849
1	-3.847751	-1.955294	-2.235958
1	-1.203434	-2.571065	-2.212158
1	-0.862999	-3.972025	1.733244
1	0.250960	2.460929	-1.663671
1	2.623790	2.922033	1.223452
1	2.461889	0.065192	2.067999
1	-1.385007	1.406465	3.421272
1	-0.401962	1.869538	4.856275
1	-0.591694	3.018009	3.480392
1	5.002382	1.175533	2.131857
1	4.419857	1.745758	3.696600
1	4.441022	-1.330347	1.508946
1	4.833791	-3.608552	2.385637
1	5.126852	-3.970116	4.845039
1	5.003446	-2.034872	6.401925
1	4.586244	0.250926	5.526020
1	3.734626	-1.893493	0.032136
1	6.190184	-2.507363	0.081661
1	6.683240	-4.098072	-0.470037
1	7.084612	-2.312809	-2.218852
1	5.992850	-3.565905	-2.799345
1	5.171013	-0.791052	-1.746293
1	5.080819	-1.338407	-3.413739
1	1.565443	-2.438842	-0.226759
1	0.472763	-6.305023	-0.762536
1	2.236989	-6.019129	-0.548684
1	1.083297	-5.366562	0.644815
1	2.295624	1.764013	-2.281643
1	3.883040	3.694858	-0.522455
1	3.009160	4.357987	-1.901466
6	4.566383	2.986423	-2.444289
6	4.040306	2.596009	-3.825379
1	5.229001	3.880772	-2.572131
6	5.180154	2.246013	-4.767765
1	3.336700	1.738481	-3.724140
1	3.441612	3.426031	-4.248934
6	6.069688	1.158161	-4.189582
1	4.773871	1.923652	-5.745780
1	5.784421	3.152070	-4.975285
6	6.580379	1.541577	-2.808985
1	5.509962	0.195774	-4.127988
1	6.921851	0.965581	-4.869094
6	5.427333	1.863305	-1.869214
1	7.186765	0.714871	-2.388648
1	7.262987	2.411169	-2.884879
1	4.821456	0.942302	-1.699662
1	5.815956	2.155707	-0.874180
8	-8.133961	-1.280926	-1.009085
6	-9.419014	-1.805131	-0.570248
6	-3.569362	-3.243607	1.736412
1	-4.075851	-2.277851	1.859838
1	-4.311537	-4.001838	1.468785
1	-3.095918	-3.521128	2.679272
1	2.845573	-1.460287	-2.273908
1	4.472848	-4.073240	0.731323
1	3.381493	-3.069051	-2.787827
8	4.206523	-4.963243	-1.141922
1	4.961204	-5.573091	-1.138897
6	-9.405894	-3.331551	-0.491457
1	-10.427380	-3.709395	-0.350204
1	-9.011945	-3.782585	-1.411610
1	-8.803223	-3.699997	0.349138
6	-9.859584	-1.188500	0.756705
1	-9.804501	-0.092176	0.733014
1	-10.901332	-1.462106	0.971069
1	-9.250519	-1.537768	1.601004
6	-10.358650	-1.349157	-1.695247
1	-11.384323	-1.683225	-1.489996
1	-10.380598	-0.255440	-1.792381
1	-10.064465	-1.764239	-2.668480

(1*R*,2*S*)$_{a,e}$-β
Et=-844.674611(-3031.092585)

6	3.676657	2.296547	-1.357541
6	2.405180	1.449295	-1.190697
6	2.263149	0.807514	0.202941
8	2.089086	-0.412057	0.342947
7	1.185021	2.210449	-1.570141
6	0.645019	3.285975	-0.805649
8	1.344742	3.804661	0.056003
6	-0.793218	3.707305	-1.141854
6	-0.889301	4.167895	-2.607007
6	-2.339555	4.522148	-2.940329
6	-3.232373	3.294257	-2.747614
6	-3.158591	2.827935	-1.281701
6	-1.701506	2.486096	-0.916638
6	-2.810223	5.657418	-2.032395
6	-2.721802	5.203110	-0.576038
6	-1.273363	4.849239	-0.232240
6	-3.623665	3.985740	-0.366755
7	-4.061296	1.648414	-1.048710
6	-3.754836	0.333284	-1.479362
8	-3.093190	0.142618	-2.488579
6	-4.354411	-0.815701	-0.642183
7	-5.830241	-0.787678	-0.833675
6	-6.636229	-1.403422	0.177410
8	-6.260381	-1.629175	1.319214
6	-3.752167	-2.186769	-0.989691
6	-2.348038	-2.392591	-0.487675
6	-1.199475	-2.690642	-1.178497
7	-0.158944	-2.898071	-0.300909
6	-0.663385	-2.736021	0.914108
7	-1.980523	-2.427651	0.857408
6	1.463375	-4.080144	-1.110787
8	2.596387	-2.739698	-0.817279
6	3.797987	-2.339037	-1.595332
6	3.478006	-1.605281	-2.904886
6	3.204825	-2.506557	-4.116948
6	4.294093	-3.575832	-4.275911
6	4.437746	-4.415372	-2.997818
6	4.753550	-3.536685	-1.786784
7	2.356476	1.618394	1.326743
6	2.084261	1.126670	2.705766
6	0.854002	1.845282	3.267656
8	0.763969	2.565213	4.234502
6	3.330954	1.340472	3.579690
6	3.379211	0.405502	4.746624
6	3.052185	-0.943514	4.594071
6	3.148226	-1.816026	5.670052
6	3.569336	-1.346737	6.910488
6	3.887895	-0.002538	7.070819
6	3.793278	0.873575	5.994323
8	-0.269615	1.587072	2.520592
6	-1.454236	2.305625	2.793054
6	1.740331	-4.967847	0.047041
8	1.166063	-4.228375	-2.233393
1	-4.278087	3.539368	-3.019511
1	-2.914598	2.486574	-3.436456
1	-2.398090	4.849859	-4.005129
1	-3.849012	5.946920	-2.284079
1	-2.191196	6.561709	-2.191675
1	-3.594999	3.681976	0.700708
1	-4.675951	4.255569	-0.586466
1	-3.062236	6.028253	0.093210
1	-0.621647	5.736469	-0.354689
1	-1.192794	4.552032	0.833612
1	-1.333270	1.633716	-1.529622
1	-1.645725	2.165449	0.150527
1	-0.532532	3.379049	-3.298135
1	-0.233132	5.045392	-2.769508
1	-4.510305	1.685230	-0.157785
1	-4.151051	-0.607490	0.447180
1	-6.101461	-0.972975	-1.777168
1	-4.399877	-2.990010	-0.581588
1	-3.733129	-2.335943	-2.084865
1	-1.064078	-2.787284	-2.246881
1	-0.120052	-2.814595	1.845787
1	0.472483	1.628579	-1.970733
1	2.239123	2.613052	1.160525
1	1.862815	0.020075	2.682766
1	-2.030938	2.148220	1.869554
1	-1.972233	1.882801	3.658776
1	-1.283959	3.378589	2.944995
1	4.248058	1.171191	2.975664
1	3.388613	2.393241	3.926003
1	2.704284	-1.297718	3.612621
1	2.893546	-2.872876	5.542339
1	3.647271	-2.034342	7.759375
1	4.213580	0.369955	8.048293
1	4.040670	1.933375	6.129569
1	0.991026	-5.762401	0.052090
1	2.744691	-5.378193	-0.103991
1	1.728504	-4.416942	0.984920
1	2.452553	0.609255	-1.943173
1	3.856928	2.948163	-0.477918
1	3.520807	2.998492	-2.205209
1	2.229180	-2.991564	-4.007236
1	3.148684	-1.881082	-5.014522
1	4.059230	-4.230351	-5.121565
1	5.254298	-3.095390	-4.511623
1	3.517214	-4.981525	-2.818499
1	5.244353	-5.148855	-3.095711
1	4.271440	-1.631556	-0.898005
1	2.642127	-0.906485	-2.729441
1	2.072659	-1.932350	-0.561340
1	4.353005	-0.959347	-3.104355
6	7.181958	1.447353	-2.741847
6	5.948921	2.278767	-2.424148
6	4.922053	1.452546	-1.645457
6	5.564065	0.925641	-0.361105
6	6.795929	0.089307	-0.672729
6	7.809582	0.889561	-1.474608
1	6.232695	3.175474	-1.837441
1	5.500452	2.659388	-3.363090
1	6.911470	0.618167	-3.426700
1	7.919830	2.063533	-3.290738
1	5.840866	1.772614	0.299338
1	4.832151	0.322795	0.213909
1	7.254556	-0.271907	0.267721
1	6.501337	-0.822496	-1.235095
1	8.208519	1.717589	-0.855116
1	8.680381	0.254946	-1.728072
1	4.635947	0.571754	-2.286747
8	-7.866234	-1.630141	-0.330708
6	-8.980129	-2.056457	0.503591
6	-2.858586	-2.228583	2.009927
1	-3.433569	-1.302271	1.885939
1	-3.554169	-3.066930	2.112793
1	-2.249813	-2.153179	2.912035
1	5.736622	-3.068772	-1.964901
8	4.808784	-4.373261	-0.637492
1	5.206982	-3.878509	0.096732
6	-10.139116	-2.108650	-0.501620
1	-11.062802	-2.422848	0.002171
1	-10.329061	-1.128298	-0.958797
1	-9.945958	-2.822866	-1.313172
6	-8.740852	-3.446364	1.092863
1	-9.664110	-3.823680	1.552630
1	-8.437609	-4.167586	0.322672
1	-7.967551	-3.440790	1.872281
6	-9.289068	-1.038394	1.600492
1	-9.392759	-0.023426	1.194710
1	-10.235404	-1.294279	2.095477
1	-8.512034	-1.012922	2.375930

(1*S*,2*R*)$_{e,a}$-α
Et= -844.674970(-3031.092368)

6	3.279111	-2.977034	-0.513803
6	4.709510	-2.999214	0.062716
6	4.913622	-4.165293	1.041986
6	4.517892	-5.508329	0.411205
6	3.089711	-5.491030	-0.155353
6	2.935386	-4.324782	-1.134676
6	1.027996	-3.571768	-3.097815
8	1.480202	-2.510589	-3.261974
6	0.571958	-4.696548	-3.955589
7	-0.933322	-3.221852	-2.007607
6	-1.524695	-2.029436	-2.357655
6	-2.858026	-2.042773	-2.019762
7	-3.071647	-3.289720	-1.440107
6	-1.897129	-3.958255	-1.463003
6	-3.946581	-1.026313	-2.247661
6	-4.177219	-0.108134	-1.030585
7	-5.619545	0.182957	-0.799222
6	-6.426286	-0.838919	-0.221335
6	-3.448869	1.249584	-1.169559
8	-2.868547	1.585135	-2.192999
7	-3.544363	2.124714	-0.067682
6	-2.685762	3.342577	0.136561
6	-3.047419	4.440246	-0.883369
6	-2.204262	5.688940	-0.615632
6	-0.717581	5.354018	-0.753097
6	-0.338193	4.266085	0.265543
6	-1.188124	3.005619	0.020146
6	-2.485234	6.211241	0.792428
6	-2.111929	5.133303	1.808760
6	-0.626288	4.795048	1.679478
6	-2.953425	3.880289	1.562401
6	1.135688	3.859661	0.113503
8	1.971378	3.950230	1.004814
7	1.536955	3.334389	-1.150078
6	2.727442	2.455173	-1.313020
6	2.634007	1.230616	-0.381862
7	2.950265	1.389254	0.983767
6	2.503358	0.382599	1.991210
6	3.716103	-0.374163	2.553930
6	3.299524	-1.434297	3.523878
6	2.571055	-2.542215	3.085194
6	2.202153	-3.537207	3.982150
6	2.555463	-3.434349	5.323772
6	3.281652	-2.333529	5.765083
6	3.654332	-1.335748	4.870093
6	4.046234	3.227550	-1.188409
8	2.308647	0.126539	-0.808722
8	-5.993509	-1.823633	0.371136
6	1.739213	1.115638	3.099233
8	0.382184	0.986537	2.956630
6	-0.462412	1.711894	3.825346
8	2.183102	1.770876	4.015449
1	-4.124620	4.689625	-0.813993
1	-2.875438	4.089730	-1.920272
1	-2.470617	6.473540	-1.362640
1	-3.552540	6.487364	0.895996
1	-1.907404	7.136314	0.983779
1	-2.705008	3.113188	2.326817
1	-4.027821	4.117964	1.693757
1	-2.311289	5.508829	2.840227
1	-0.007814	5.690569	1.885416
1	-0.338129	4.040177	2.446366
1	-0.954949	2.598614	-0.989006
1	-0.913744	2.219259	0.753435
1	-0.506147	5.023472	-1.789134
1	-0.103142	6.259945	-0.583830
1	-3.811632	1.684629	0.787051
1	-3.788568	-0.618892	-0.111982
1	-6.041619	0.710115	-1.535289
1	-4.880898	-1.552883	-2.523197
1	-3.669685	-0.434196	-3.140309
1	-0.962028	-1.235709	-2.831458
1	-1.788924	-4.962267	-1.076097
1	0.754388	3.012228	-1.688465
1	2.930534	2.355410	1.295071
1	1.823789	-0.369413	1.505983
1	-1.456460	1.359062	3.535768
1	-0.268807	1.494004	4.880650
1	-0.376326	2.793912	3.637963
1	4.273624	-0.858986	1.715796
1	4.429624	0.329331	3.029361
1	2.295423	-2.629796	2.020849
1	1.631970	-4.402978	3.628779
1	2.262009	-4.217536	6.030638
1	3.560766	-2.249082	6.821109
1	4.221990	-0.466517	5.225180
1	5.437901	-3.064271	-0.757053
1	4.599659	-6.325851	1.139749
1	5.207564	-5.761864	-0.405937
1	4.307261	-3.990779	1.942791
1	5.958093	-4.205726	1.368221
1	-0.043055	-4.281171	-4.757441
1	1.463855	-5.160502	-4.394292
1	0.016498	-5.436954	-3.386886
1	2.679180	2.081180	-2.378069
1	4.301566	3.443442	-0.130669
1	3.940126	4.222292	-1.670018
1	4.888100	-2.039287	0.573935
6	6.131262	1.609617	-4.017284
6	4.993790	2.376106	-3.363963
6	5.194006	2.462084	-1.849835
6	6.531115	3.136337	-1.543260
6	7.677413	2.382383	-2.199954
6	7.469606	2.259981	-3.701539
1	4.927046	3.395158	-3.795826
1	4.013855	1.893331	-3.576444
1	6.129284	0.557637	-3.668653
1	5.978037	1.565879	-5.112576
1	6.513233	4.186776	-1.897341
1	6.689787	3.188011	-0.448285
1	8.634592	2.897749	-1.991098
1	7.772495	1.374202	-1.749233
1	7.520104	3.262518	-4.171424
1	8.292723	1.672996	-4.152121
1	5.219396	1.423476	-1.434628
1	3.524779	-4.517451	-2.035282
8	1.525193	-4.381072	-1.611802
1	0.929739	-4.012932	-0.925863
1	3.173134	-2.180481	-1.257295
1	2.884186	-6.432293	-0.686903
1	2.570890	-2.769245	0.307419
8	2.086224	-5.266360	0.836691
1	2.241481	-5.861717	1.586874
8	-7.724505	-0.514307	-0.387978
6	-8.798772	-1.255943	0.257029
6	-4.337408	-3.826547	-0.951667
1	-4.867911	-3.075448	-0.330192
1	-4.979173	-4.116260	-1.788880
1	-4.134691	-4.707534	-0.340750
6	-8.877560	-2.692056	-0.260698
1	-8.893448	-2.728230	-1.357895
1	-8.035485	-3.306439	0.084498
1	-9.798626	-3.170587	0.098225
6	-10.044058	-0.474032	-0.183491
1	-10.014493	0.569191	0.158630
1	-10.156638	-0.463250	-1.275882
1	-10.947865	-0.934258	0.237319
6	-8.676259	-1.223791	1.779701
1	-7.833257	-1.826231	2.143203
1	-8.544262	-0.200207	2.154531
1	-9.588196	-1.628246	2.238939

(1*S*,2*R*)$_{e,a}$-β

Et=-844.682585 (-3031.0887569)

6	3.550846	3.254540	-1.391972
6	2.403433	2.238896	-1.292280
6	2.492747	1.299736	-0.074951
8	2.379963	0.078954	-0.207294
7	1.068472	2.903410	-1.333836
6	0.565011	3.685854	-0.252870
8	1.360262	4.130034	0.567458
6	-0.952979	3.911778	-0.193432
6	-1.443338	4.664493	-1.441334
6	-2.963595	4.828902	-1.376648
6	-3.637292	3.455565	-1.327985
6	-3.160467	2.689861	-0.078200
6	-1.630061	2.530536	-0.124581
6	-3.338865	5.633664	-0.132979
6	-2.857935	4.887194	1.110477
6	-3.528949	3.515070	1.178077
6	-1.339584	4.718167	1.057076
7	-3.790967	1.333105	0.072442
6	-3.749843	0.318040	-0.915737
8	-3.053517	0.418025	-1.914693
6	-4.553823	-0.955112	-0.579269
7	-5.987275	-0.648802	-0.842417
6	-6.964671	-1.444382	-0.155983
8	-6.745539	-2.092722	0.856256
6	-4.066453	-2.182648	-1.365785
6	-2.719032	-2.678456	-0.917992
6	-1.517760	-2.715280	-1.581641
7	-0.555224	-3.308811	-0.796511
6	-1.161839	-3.634881	0.336378
7	-2.468629	-3.273092	0.315189
6	1.363289	-3.684549	-2.012215
6	1.423191	-5.157766	-1.908597
8	1.252194	-2.851265	-2.813465
7	2.716851	1.851748	1.192592
6	2.548422	1.050451	2.437962
6	1.524766	1.752624	3.336355
8	1.716565	2.567286	4.210928
6	3.905929	0.875680	3.144761
6	3.995642	-0.472947	3.784412
6	4.060465	-1.611959	2.980210
6	4.145161	-2.874512	3.552712
6	4.174836	-3.009721	4.936619
6	4.117878	-1.877203	5.742778
6	4.026871	-0.611128	5.172071
8	0.242480	1.367388	3.044106
6	-0.828555	2.049940	3.662406
6	4.179835	-2.348761	-1.820210
6	5.632236	-1.874436	-1.680618
6	6.520812	-2.956104	-1.049403
6	5.946796	-3.457279	0.285072
6	4.471300	-3.901999	0.169072
6	3.664460	-2.765235	-0.446308
8	2.216642	-3.137697	-0.483051
1	-4.738470	3.576614	-1.310029
1	-3.400413	2.893012	-2.252652
1	-3.309540	5.370837	-2.288372
1	-4.434176	5.790558	-0.090353
1	-2.884764	6.642789	-0.175068
1	-3.207800	2.986226	2.099879
1	-4.627597	3.642626	1.256971
1	-3.127408	5.470675	2.022430
1	-0.841716	5.707400	1.044564
1	-0.981030	4.202847	1.977793
1	-1.323638	1.926981	-1.007652
1	-1.277884	1.982729	0.774516
1	-1.165796	4.122497	-2.366811
1	-0.953909	5.656279	-1.501796
1	-4.654493	1.363020	0.573029
1	-4.445661	-1.179663	0.521279
1	-6.171240	-0.496229	-1.812833
1	-4.809444	-3.001281	-1.277636
1	-3.991908	-1.948887	-2.443730
1	-1.291267	-2.337389	-2.569634
1	-0.702256	-4.116854	1.188371
1	0.360603	2.323675	-1.745009
1	2.519570	2.845300	1.262330
1	2.154020	0.032386	2.173060
1	-1.697975	1.483299	3.315885
1	-0.767230	2.031943	4.755391
1	-0.887446	3.089131	3.300493
1	4.737699	0.974558	2.416195
1	4.074681	1.677491	3.892901
1	4.048519	-1.508007	1.882975
1	4.194892	-3.756735	2.895250
1	4.248056	-4.003755	5.390109
1	4.146628	-1.980796	6.833121
1	3.982639	0.277715	5.813362
1	3.704922	-1.895034	0.228928
1	6.013734	-2.658119	1.039015
1	6.543119	-4.292247	0.667176
1	7.531937	-2.564062	-0.897446
1	6.607078	-3.796588	-1.747784
1	5.632030	-0.941590	-1.083198
1	6.006611	-1.576762	-2.675509
1	1.669848	-2.352436	-0.281018
1	0.673109	-5.571636	-2.587049
1	2.425843	-5.450018	-2.238164
1	1.246012	-5.487843	-0.888798
1	2.447928	1.600184	-2.222088
1	3.884614	3.591667	-0.389228
1	3.171878	4.170934	-1.893401
6	4.771657	2.774726	-2.179613
6	4.401660	2.255629	-3.568264
1	5.421806	3.677632	-2.316608
6	5.646017	1.902630	-4.367137
1	3.728307	1.374373	-3.465314
1	3.810871	3.019152	-4.111634
6	6.544042	0.928418	-3.622586
1	5.355195	1.476101	-5.346457
1	6.212635	2.827495	-4.597420
6	6.875866	1.431070	-2.225537
1	6.055453	-0.070817	-3.551669
1	7.476300	0.762628	-4.196124
6	5.607759	1.732137	-1.438359
1	7.482503	0.675794	-1.687578
1	7.509226	2.338221	-2.288997
1	5.041140	0.783867	-1.281276
1	5.863831	2.100053	-0.425674
8	-8.150838	-1.301272	-0.785419
6	-9.388873	-1.826707	-0.228825
6	-3.439643	-3.476541	1.387799
1	-3.994345	-2.544996	1.564339
1	-4.147977	-4.267775	1.124352
1	-2.911525	-3.757093	2.300368
1	3.555339	-1.532263	-2.214781
1	4.072897	-4.133309	1.170669
1	4.390018	-4.800201	-0.451087
8	4.069736	-3.506227	-2.657005
1	4.297528	-3.245996	-3.563420
6	-10.430547	-1.366392	-1.258162
1	-10.461178	-0.272317	-1.348613
1	-10.229923	-1.777748	-2.256438
1	-11.432350	-1.701210	-0.958116
6	-9.369436	-3.353414	-0.157084
1	-8.689846	-3.725211	0.621063
1	-10.373114	-3.731402	0.079389
1	-9.065158	-3.801312	-1.112130
6	-9.701489	-1.214773	1.136078
1	-9.015443	-1.567272	1.917680
1	-9.648214	-0.118392	1.111235
1	-10.718428	-1.488863	1.447148

(1*S*,2*R*)$_{a,e}$-β

Et=-844.686694(-3031.105557)

6	-6.852949	2.544871	-3.628718
6	-5.550342	2.918971	-2.939021
6	-4.524598	1.807771	-3.088198
6	-5.061888	0.493876	-2.518165
6	-6.352506	0.112494	-3.242249
6	-7.387945	1.219203	-3.109293
6	-4.021776	-0.621904	-2.640734
6	-2.830541	-0.353616	-1.710108
6	-3.150232	-0.662634	-0.233445
8	-3.012035	0.198259	0.646474
7	-1.587679	-1.018520	-2.179727
6	-1.321864	-2.408790	-2.049254
8	-2.264216	-3.167768	-1.851580
6	0.137495	-2.862371	-2.214735
6	0.548497	-2.718154	-3.690054
6	2.004513	-3.152831	-3.864109
6	2.913863	-2.265585	-3.012975
6	2.523468	-2.396489	-1.527535
6	1.051241	-1.990491	-1.332563
6	2.161043	-4.612511	-3.439596
6	1.764010	-4.753370	-1.970585
6	0.305854	-4.330749	-1.790211
6	2.672437	-3.877989	-1.105923
7	3.389048	-1.568060	-0.616849
6	3.621414	-0.179501	-0.789730
8	2.924366	0.499355	-1.528616
6	4.723133	0.423317	0.105883
7	6.027113	-0.116455	-0.373400
6	7.108032	-0.156137	0.570564
8	6.971614	-0.114766	1.783987
6	4.712887	1.960804	0.121601
6	3.561496	2.557752	0.883737
6	2.547849	3.379838	0.456220
7	1.750019	3.736395	1.518042
6	2.268839	3.146640	2.586230
7	3.364692	2.422455	2.256344
7	-3.657066	-1.915289	0.107591
6	-3.735251	-2.386186	1.519432
6	-2.570071	-3.340497	1.804777
8	-2.594638	-4.510602	2.110537
6	-5.097950	-3.055778	1.756109
6	-5.490211	-3.062493	3.199912
6	-5.292252	-1.934239	3.998599
6	-5.705775	-1.930673	5.324245
6	-6.318939	-3.056825	5.864634
6	-6.511250	-4.186266	5.076502
6	-6.098363	-4.192486	3.748159
8	8.264569	-0.301410	-0.110803
8	-1.353988	-2.717492	1.668693
6	-0.179923	-3.498942	1.709704
6	0.348150	5.359870	1.092617
8	0.476901	5.544245	-0.062692
6	0.603517	6.197006	2.298984
8	-0.885032	4.293810	1.549466
6	-2.333663	4.366593	1.153444
6	-2.478247	3.443639	-0.077779
6	-2.233407	4.132735	-1.417461
6	-3.037666	5.436592	-1.533795
6	-2.671602	6.413370	-0.406518
6	-2.889404	5.777192	0.977713
1	3.972121	-2.559048	-3.160450
1	2.830522	-1.215106	-3.355276
1	2.290922	-3.045076	-4.936946
1	3.204970	-4.948843	-3.591992
1	1.531068	-5.267517	-4.072382
1	2.408581	-4.006599	-0.035885
1	3.723380	-4.215075	-1.212155
1	1.875921	-5.817584	-1.654929
1	-0.359083	-4.983363	-2.389425
1	-0.005021	-4.464461	-0.728245
1	0.907310	-0.916884	-1.584394
1	0.768144	-2.108162	-0.259234
1	0.424428	-1.670941	-4.029720
1	-0.112930	-3.335331	-4.329293
1	4.194943	-2.067742	-0.303282
1	4.563642	0.053769	1.159306
1	6.270087	0.228859	-1.279238
1	5.665894	2.333448	0.550601
1	4.664000	2.358184	-0.908745
1	2.343086	3.730919	-0.546051
1	1.890125	3.209413	3.596919
1	-0.771837	-0.447527	-2.059686
1	-3.505189	-2.638086	-0.588112
1	-3.653297	-1.506618	2.222029
1	0.582973	-2.780939	1.375356
1	0.028658	-3.860835	2.720315
1	-0.215244	-4.342477	1.000770
1	-5.888906	-2.511644	1.198379
1	-5.099901	-4.088983	1.350960
1	-4.791218	-1.056404	3.564233
1	-5.549328	-1.041404	5.943144
1	-6.647194	-3.054252	6.909289
1	-6.988409	-5.075719	5.501874
1	-6.248053	-5.088487	3.134133
1	1.594448	6.644709	2.200003
1	-0.144254	6.998933	2.318282
1	0.532841	5.615652	3.215538
1	-2.610534	0.753196	-1.792068
1	-4.493962	-1.603474	-2.432038
1	-3.671102	-0.687150	-3.692015
1	-1.162708	4.337616	-1.522570
1	-2.511734	3.420482	-2.210853
1	-2.848218	5.898311	-2.508056
1	-4.115203	5.210799	-1.502565
1	-1.630995	6.730321	-0.528174
1	-3.285385	7.318198	-0.470892
1	-2.533932	6.420905	1.791174
1	-3.970245	5.672543	1.145277
1	-2.801965	3.894328	2.022829
1	-0.626794	3.397237	1.164143
1	-4.257324	1.677688	-4.156100
1	-3.571521	2.082063	-2.569620
1	-5.729399	3.125098	-1.863582
1	-5.148907	3.862315	-3.359683
1	-6.140318	-0.087022	-4.311888
1	-6.755123	-0.833790	-2.830872
1	-8.307010	0.941375	-3.660313
1	-7.692121	1.325031	-2.048613
1	-6.692230	2.483180	-4.723640
1	-7.604909	3.342892	-3.477592
1	-5.298759	0.646136	-1.434915
6	9.528733	-0.566324	0.560855
6	4.205787	1.671920	3.186802
1	4.382053	0.660568	2.797355
1	5.169171	2.171820	3.325340
1	3.696971	1.600205	4.149265
6	9.950276	0.605234	1.447374
1	10.985923	0.466806	1.785702
1	9.904763	1.560260	0.907770
1	9.323960	0.695049	2.344730
6	9.485809	-1.871118	1.355031
1	10.494744	-2.135363	1.698987
1	8.847241	-1.796324	2.245234
1	9.116063	-2.705786	0.745004
6	10.501704	-0.704511	-0.618366
1	11.515459	-0.910307	-0.249965
1	10.219840	-1.528436	-1.287562
1	10.548897	0.212638	-1.220562
1	-3.496401	3.031033	-0.061807
8	-1.513415	2.388276	0.090218
1	-1.960962	1.570479	0.419922

(1*S*,2*S*)$_{e,e}$-α

Et=-844.689557 (−3031.0861334)

6	3.745201	-1.969675	0.496462
6	5.127486	-1.299991	0.512777
6	6.245201	-2.346411	0.421263
6	6.046176	-3.216363	-0.831063
6	4.671849	-3.904822	-0.845614
6	3.583486	-2.846671	-0.737492
6	1.471671	-3.885932	-2.303155
8	1.628438	-3.025020	-3.069207
6	1.370107	-5.361573	-2.279504
7	-0.425619	-3.370970	-1.261538
6	-1.277397	-2.543009	-1.956690
6	-2.549288	-2.632041	-1.441449
7	-2.454714	-3.550280	-0.398408
6	-1.170067	-3.965094	-0.334522
6	-3.834998	-1.978437	-1.874446
6	-4.231574	-0.784501	-0.983336
7	-5.705990	-0.669437	-0.809545
6	-6.342867	-1.585081	0.079089
6	-3.712668	0.565288	-1.529327
8	-3.142846	0.665176	-2.606427
7	-3.980541	1.707949	-0.739915
6	-3.202620	2.992571	-0.828629
6	-3.533100	3.745438	-2.131874
6	-2.764490	5.068365	-2.170156
6	-1.258648	4.800164	-2.120866
6	-0.910597	4.058285	-0.819760
6	-1.687736	2.730647	-0.754589
6	-3.170305	5.937327	-0.980708
6	-2.829289	5.202379	0.314691
6	-1.324645	4.933633	0.373620
6	-3.598242	3.881330	0.374186
6	0.584990	3.711454	-0.767964
8	1.363345	4.122751	0.083602
7	1.083373	2.834127	-1.779714
6	2.241899	1.931168	-1.546353
6	2.080991	1.138550	-0.234526
7	2.389136	1.766187	0.977980
6	2.111706	1.119827	2.294036
6	3.437010	0.876070	3.035527
6	3.246383	-0.046412	4.197376
6	3.168480	-1.425791	3.993212
6	3.008054	-2.284145	5.073950
6	2.927600	-1.773340	6.365547
6	3.010196	-0.400869	6.573795
6	3.169975	0.462195	5.494697
6	3.584825	2.664824	-1.652235
8	1.733055	-0.046305	-0.247989
8	-5.761364	-2.252788	0.929680
6	1.164307	2.033207	3.078620
8	-0.150114	1.744356	2.820144
6	-1.147325	2.604176	3.330858
8	1.439784	2.940553	3.831253
1	-4.622052	3.938356	-2.197818
1	-3.271490	3.136239	-3.019596
1	-3.007314	5.601544	-3.119541
1	-4.252947	6.166164	-1.021657
1	-2.647403	6.912751	-1.018339
1	-3.376559	3.368532	1.334554
1	-4.688337	4.080300	0.369031
1	-3.120308	5.832492	1.188172
1	-0.762118	5.887705	0.361102
1	-1.062800	4.435052	1.334958
1	-1.366056	2.074459	-1.594222
1	-1.436574	2.195005	0.184383
1	-0.956501	4.211539	-3.009436
1	-0.697330	5.753622	-2.173130
1	-4.266352	1.497638	0.192992
1	-3.786598	-0.928759	0.035525
1	-6.191780	-0.475710	-1.660534
1	-4.641009	-2.738388	-1.887867
1	-3.710281	-1.660301	-2.926189
1	-0.929046	-1.936042	-2.781489
1	-0.823803	-4.686449	0.392717
1	0.341772	2.362351	-2.263546
1	2.345022	2.779984	0.949853
1	1.617155	0.123594	2.138990
1	-2.069474	2.090077	3.044439
1	-1.091442	2.718037	4.418299
1	-1.098356	3.589589	2.840939
1	4.179750	0.421192	2.334516
1	3.882418	1.834651	3.370913
1	3.247949	-1.836819	2.973554
1	2.951047	-3.364931	4.909285
1	2.804120	-2.451259	7.216775
1	2.951894	0.003841	7.590142
1	3.234813	1.544695	5.663048
1	5.209523	-0.608925	-0.352617
1	6.829714	-3.981114	-0.904576
1	6.122213	-2.580236	-1.731237
1	6.247598	-2.975158	1.321957
1	7.222266	-1.853533	0.375524
1	0.704083	-5.668963	-3.089686
1	2.386269	-5.730567	-2.453901
1	1.007132	-5.721655	-1.320691
1	2.227706	1.181897	-2.391539
1	3.738574	3.369375	-0.809141
1	3.584570	3.297648	-2.564258
1	5.210564	-0.683124	1.421774
6	5.816690	-0.198769	-2.982303
6	4.679559	0.809318	-2.975524
6	4.748138	1.674816	-1.716047
6	6.087440	2.409753	-1.671502
6	7.242021	1.418916	-1.702326
6	7.160715	0.510702	-2.920062
1	4.728311	1.447149	-3.880813
1	3.691662	0.298088	-3.019252
1	5.713285	-0.895281	-2.110566
1	5.759363	-0.834660	-3.885737
1	6.162192	3.110829	-2.526980
1	6.149167	3.035647	-0.759791
1	8.205462	1.963755	-1.699839
1	7.238297	0.805924	-0.777023
1	7.316087	1.102820	-3.843892
1	7.980747	-0.232503	-2.894904
1	4.694978	0.991306	-0.822829
1	3.581592	-2.233947	-1.648343
8	2.270042	-3.522725	-0.669459
1	1.599674	-2.880304	-0.353376
1	2.946031	-1.194073	0.487994
1	3.608049	-2.569860	1.411970
8	-7.672856	-1.547854	-0.136891
6	-8.621112	-2.220880	0.740013
6	-3.545046	-4.072446	0.420946
1	-4.255131	-3.266355	0.698705
1	-4.089058	-4.851861	-0.120833
1	-3.127809	-4.500742	1.333706
1	4.586258	-4.581845	0.019514
8	4.441948	-4.623766	-2.058365
1	5.202979	-5.205259	-2.214707
6	-9.970012	-1.831734	0.119460
1	-10.122095	-0.744017	0.119436
1	-10.060345	-2.180783	-0.917900
1	-10.792774	-2.280323	0.691833
6	-8.537548	-1.697892	2.173193
1	-7.612629	-2.008135	2.677171
1	-8.588442	-0.601624	2.208723
1	-9.377350	-2.086430	2.764709
6	-8.447001	-3.738716	0.694599
1	-7.524322	-4.067490	1.190742
1	-9.285215	-4.228283	1.208363
1	-8.427666	-4.115041	-0.336614

(1*S*,2*S*)$_{e,e}$-β

Et=-844.690905 (-3031.1003428)

6	3.549576	3.196177	-1.863000
6	2.398343	2.256933	-1.469409
6	2.702728	1.412539	-0.220378
8	2.611913	0.176948	-0.247813
7	1.098602	2.969474	-1.349153
6	0.731397	3.759247	-0.221751
8	1.620121	4.233356	0.476360
6	-0.772586	3.952695	0.024557
6	-1.412946	4.730316	-1.137629
6	-2.918488	4.861158	-0.898597
6	-3.555008	3.472564	-0.820744
6	-2.931122	2.679187	0.345037
6	-1.413304	2.555158	0.132691
6	-3.168734	5.617178	0.405804
6	-2.535670	4.844965	1.562784
6	-3.168583	3.455914	1.662174
6	-1.029308	4.718216	1.331422
7	-3.538489	1.311054	0.501894
6	-3.570520	0.335890	-0.530236
8	-2.846390	0.412347	-1.510852
6	-4.509057	-0.862921	-0.282184
7	-5.862592	-0.432137	-0.732724
6	-6.991242	-1.121998	-0.177731
8	-6.967549	-1.769429	0.858735
6	-4.040361	-2.145137	-0.990839
6	-2.879882	-2.825630	-0.316434
6	-1.621559	-3.120198	-0.786781
7	-0.913387	-3.816752	0.168054
6	-1.728427	-3.957329	1.202299
7	-2.928160	-3.379611	0.960259
6	0.954209	-4.856655	-0.313407
6	1.059934	-5.678545	0.923726
8	0.906457	-5.100834	-1.461526
7	3.116822	2.027452	0.956207
6	3.288701	1.251209	2.219168
6	2.609256	2.005603	3.365636
8	3.114182	2.626247	4.273929
6	4.785436	0.996760	2.481487
6	5.009474	-0.377281	3.029202
6	4.805605	-1.494419	2.216547
6	5.033316	-2.772962	2.711017
6	5.469399	-2.947284	4.019948
6	5.673649	-1.837513	4.833497
6	5.444647	-0.555736	4.342989
8	1.244395	1.911983	3.289792
6	0.459360	2.619146	4.227401
6	2.810639	-2.598342	-1.960719
6	4.104960	-2.029955	-2.534601
6	5.213226	-3.100697	-2.477845
6	5.409316	-3.672932	-1.061777
6	4.093625	-4.201014	-0.440483
6	3.074651	-3.080672	-0.531825
8	1.749396	-3.380805	0.082654
1	-4.650032	3.568318	-0.680478
1	-3.408808	2.939917	-1.781500
1	-3.374165	5.423536	-1.747558
1	-4.255446	5.745685	0.575173
1	-2.743671	6.638061	0.346907
1	-2.733224	2.906595	2.522180
1	-4.252774	3.556844	1.871439
1	-2.712132	5.394448	2.517523
1	-0.561810	5.721584	1.285781
1	-0.552034	4.195000	2.185855
1	-1.194898	1.977488	-0.792881
1	-0.955488	1.995315	0.973594
1	-1.231790	4.221435	-2.104908
1	-0.950502	5.733336	-1.221758
1	-4.383912	1.342140	1.032969
1	-4.570631	-1.069198	0.824335
1	-5.903704	-0.274830	-1.718933
1	-4.885833	-2.860150	-1.061684
1	-3.737070	-1.927817	-2.031687
1	-1.185755	-2.867377	-1.744669
1	-1.500267	-4.459359	2.131743
1	0.335443	2.416442	-1.693931
1	2.905524	3.016980	1.030606
1	2.774972	0.256206	2.119340
1	-0.556593	2.431866	3.863977
1	0.588792	2.221631	5.239140
1	0.675891	3.693657	4.217793
1	5.367395	1.094488	1.540752
1	5.206007	1.762159	3.166155
1	4.463411	-1.365239	1.176418
1	4.871937	-3.642194	2.053517
1	5.656767	-3.953967	4.407787
1	6.019833	-1.971451	5.864335
1	5.609751	0.315540	4.989083
1	3.425184	-2.230334	0.084165
1	5.815713	-2.892449	-0.402215
1	6.147121	-4.481081	-1.078917
1	6.153904	-2.667543	-2.835089
1	4.960604	-3.914659	-3.170413
1	4.408174	-1.138944	-1.948052
1	3.951088	-1.677166	-3.566366
1	1.177546	-2.688357	-0.352748
1	0.309355	-6.470376	0.873791
1	2.054791	-6.138400	0.938029
1	0.932976	-5.071873	1.817853
1	2.244296	1.544534	-2.333378
1	4.132684	3.514131	-0.975308
1	3.131728	4.133379	-2.287547
6	4.506143	2.594724	-2.899020
6	3.770165	2.200396	-4.180627
1	5.244363	3.394941	-3.160305
6	4.724112	1.627476	-5.215090
1	2.975208	1.458477	-3.938150
1	3.243050	3.080666	-4.597456
6	5.500526	0.448709	-4.653036
1	4.160292	1.317511	-6.115938
1	5.427888	2.413962	-5.554250
6	6.247475	0.846997	-3.389455
1	4.807164	-0.396764	-4.430251
1	6.210385	0.064497	-5.409978
6	5.293181	1.407157	-2.345709
1	6.780992	-0.031499	-2.974799
1	7.029770	1.593809	-3.630141
1	4.601283	0.597845	-2.012913
1	5.853731	1.714986	-1.441323
8	-8.066476	-0.881517	-0.957806
6	-9.410249	-1.281651	-0.566122
6	-4.073763	-3.392122	1.868138
1	-4.470673	-2.375313	1.986318
1	-4.865870	-4.039517	1.480000
1	-3.751228	-3.764129	2.841608
1	4.265362	-4.471680	0.614225
1	2.468754	-3.438942	-2.569588
1	3.747549	-5.088994	-0.982806
8	1.692499	-1.701575	-1.914685
1	2.004381	-0.830755	-1.564468
6	-9.542475	-2.802187	-0.484108
1	-10.599304	-3.082463	-0.380467
1	-9.158536	-3.292912	-1.388052
1	-9.008520	-3.220837	0.379130
6	-9.839851	-0.619492	0.742349
1	-9.681744	0.466766	0.718696
1	-10.909816	-0.793505	0.918315
1	-9.297716	-1.019538	1.609435
6	-10.260993	-0.746123	-1.726212
1	-11.320215	-0.982294	-1.558793
1	-10.177417	0.344369	-1.826031
1	-9.970960	-1.191885	-2.687054

$(1S,2S)_{a,a}$-β

Et=-844.669115 (-3031.095514)

6	-6.709810	1.709722	-4.555869
6	-5.489492	2.261891	-3.835607
6	-4.434955	1.182844	-3.657075
6	-5.003879	-0.014168	-2.892367
6	-6.216287	-0.573968	-3.635704
6	-7.274898	0.501799	-3.824841
6	-3.941665	-1.100749	-2.709312
6	-2.822447	-0.620065	-1.774848
6	-3.221270	-0.682642	-0.287062
8	-3.195230	0.330215	0.422516
7	-1.530229	-1.301790	-2.050001
6	-1.246494	-2.655674	-1.729720
8	-2.179393	-3.402507	-1.454970
6	0.222096	-3.103935	-1.804631
6	0.656221	-3.153060	-3.279716
6	2.118371	-3.590989	-3.372358
6	3.005057	-2.588536	-2.632628
6	2.591341	-2.526964	-1.149009
6	1.113059	-2.111468	-1.033435
6	2.279896	-4.979710	-2.755073
6	1.859253	-4.929452	-1.286658
6	0.395803	-4.500563	-1.184601
6	2.744991	-3.937894	-0.531750
7	3.446219	-1.583255	-0.346115
6	3.678049	-0.229459	-0.694128
8	2.953371	0.363552	-1.479749
6	4.820272	0.465418	0.076145
7	6.101802	-0.103578	-0.427434
6	7.241492	-0.020582	0.442355
8	7.178946	0.159244	1.649362
6	4.784390	1.997290	-0.046874
6	3.649732	2.634258	0.706837
6	2.584709	3.369754	0.250259
7	1.810065	3.789349	1.309399
6	2.401591	3.323857	2.404147
7	3.514360	2.620713	2.093549
7	-3.657202	-1.893078	0.252390
6	-3.764937	-2.119046	1.720860
6	-2.603076	-3.006173	2.181545
8	-2.628334	-4.111948	2.671083
6	-5.129730	-2.747645	2.042835
6	-5.544257	-2.518721	3.462023
6	-5.369398	-1.270242	4.062772
6	-5.803551	-1.049584	5.363188
6	-6.413977	-2.076672	6.076439
6	-6.583157	-3.324445	5.486392
6	-6.149898	-3.548144	4.183578
8	8.355003	-0.227289	-0.291526
8	-1.384599	-2.405819	1.973528
6	-0.212312	-3.170959	2.150484
6	0.371158	5.414969	0.789992
8	0.512456	5.534223	-0.360168
6	0.491294	6.264099	2.000145
8	-0.863150	4.193531	1.287365
6	-2.298246	3.985620	0.875419
6	-2.443211	3.367719	-0.533306
6	-2.319876	4.382700	-1.673140
6	-3.222629	5.606608	-1.455533
6	-2.928850	6.280838	-0.106936
6	-3.077048	5.283337	1.054880
8	-3.750622	2.815427	-0.585174
1	4.068322	-2.886584	-2.724782
1	2.917185	-1.592383	-3.109861
1	2.422054	-3.623529	-4.445358
1	3.328949	-5.322490	-2.845213
1	1.665986	-5.719185	-3.305198
1	2.463532	-3.925477	0.541368
1	3.800242	-4.275761	-0.575293
1	1.974812	-5.941441	-0.831410
1	-0.254838	-5.234337	-1.699844
1	0.069056	-4.492578	-0.118760
1	0.962010	-1.084098	-1.431067
1	0.811991	-2.085442	0.040898
1	0.527755	-2.161873	-3.757717
1	0.010899	-3.857165	-3.840909
1	4.254963	-2.036330	0.026227
1	4.731784	0.194169	1.167357
1	6.277739	0.140760	-1.380381
1	5.745294	2.422255	0.308887
1	4.686918	2.299502	-1.105617
1	2.331114	3.619059	-0.771392
1	2.063010	3.466253	3.421068
1	-0.734713	-0.698344	-1.960796
1	-3.443427	-2.713686	-0.304036
1	-3.699104	-1.133819	2.267624
1	0.560705	-2.502491	1.744815
1	-0.030074	-3.395593	3.205167
1	-0.229523	-4.101069	1.558637
1	-5.912290	-2.305593	1.390961
1	-5.123395	-3.833156	1.812374
1	-4.871594	-0.471636	3.492871
1	-5.666793	-0.066934	5.825697
1	-6.759089	-1.902863	7.100979
1	-7.058743	-4.135563	6.048187
1	-6.282176	-4.535807	3.726114
1	1.432137	6.815932	1.932100
1	-0.344005	6.974303	1.986225
1	0.448846	5.673189	2.911166
1	-2.634039	0.465443	-2.032544
1	-4.415476	-2.030979	-2.334957
1	-3.516800	-1.369378	-3.699225
1	-1.274836	4.696981	-1.767715
1	-2.590295	3.861706	-2.598699
1	-3.080728	6.321299	-2.273095
1	-4.272207	5.290356	-1.486181
1	-1.918876	6.712156	-0.127890
1	-3.614572	7.118562	0.059872
1	-2.826895	5.731357	2.024031
1	-4.128068	4.977189	1.118195
1	-2.629377	3.247508	1.614707
1	-1.683701	2.576345	-0.660877
1	-0.339411	3.377354	1.163840
1	-3.735148	1.910215	-0.199447
1	-4.052589	0.856219	-4.644960
1	-3.554036	1.584834	-3.105338
1	-5.781071	2.671461	-2.847303
1	-5.064348	3.113376	-4.401111
1	-5.901977	-0.977237	-4.619405
1	-6.642757	-1.430855	-3.078337
1	-8.134776	0.087759	-4.385718
1	-7.677250	0.811819	-2.839615
1	-6.439887	1.429768	-5.593737
1	-7.484535	2.495048	-4.645937
1	-5.338099	0.337090	-1.883412
6	9.665165	-0.393396	0.322153
6	4.425726	1.993128	3.050380
1	4.628515	0.957916	2.746108
1	5.370852	2.542047	3.097329
1	3.960976	1.991672	4.037342
6	10.115213	0.879789	1.037970
1	11.173008	0.797177	1.321663
1	10.014512	1.764562	0.395818
1	9.545032	1.064318	1.957971
6	9.701394	-1.597106	1.262622
1	10.735702	-1.804432	1.568149
1	9.118863	-1.428511	2.178066
1	9.312703	-2.502645	0.778425
6	10.563908	-0.653508	-0.894664
1	11.603386	-0.799852	-0.572372
1	10.258707	-1.553949	-1.444392
1	10.552263	0.187820	-1.600410