Supplementary Information (SI) for Organic Chemistry Frontiers.

Supporting Information

Electronic Structure Origins of Radical Character in Triangular Acenes: Sextet Stabilization vs. Antiaromaticity Release

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Table S1. Energy and <S2> considerations on DFT-optimized An and Tn series obtained at the M06-2X/6-311+G(d,p) computational level.

	Linear, An			**Triangular, Tn**		
n	$\Delta E_{UKS-RKS}$[a]	<S2>[b]	ΔE_{S-T}[c]	$\Delta E_{UKS-RKS}$[a]	<S2>[b]	ΔE_{S-T}[c]
3	-	-	2.03	-	0.03	0.63
4	-	-	1.42	0.001	1.70	0.44
5	-	-	0.96	2.3	2.76	0.41
6	-	-	0.64	7.5	3.51	0.41
7	1.34	0.44	0.45	14.0	0.03	0.69

[a]UKS-RKS stability differences in kcal/mol. [b] Expectation value of the S^2 upon UKS optimization. [c]Adiabatic vertical spin flip excitation energy between singlet and triplet states in eV.

Table S2. HOMO-LUMO energy gaps in eV of An and Tn series computed at the M06-2X/6-311+G(d,p) level.

n	An	Tn
3	5.48	3.24
4	4.56	2.79
5	3.90	2.75
6	3.41	2.73
7	3.37	2.97

Table S3. Calculated adiabatic (adiab) and vertical (vert) singlet-triplet energy gaps (in eV) computed at the M06-2X and RAS-SF levels for the An and Tn series.

	M06-2X, adiab		M06-2X, vert		RAS-SF, vert	
n	An	Tn	An	Tn	An	Tn
3	2.03	0.63	2.50	1.09	2.50	1.14
4	1.42	0.44	1.82	0.85	1.95	0.96
5	0.96	0.41	1.33	0.79	1.45	0.67
6	0.64	0.41	0.97	0.80	1.11	0.47
7	0.45	0.69	0.64	0.91	0.72	0.31

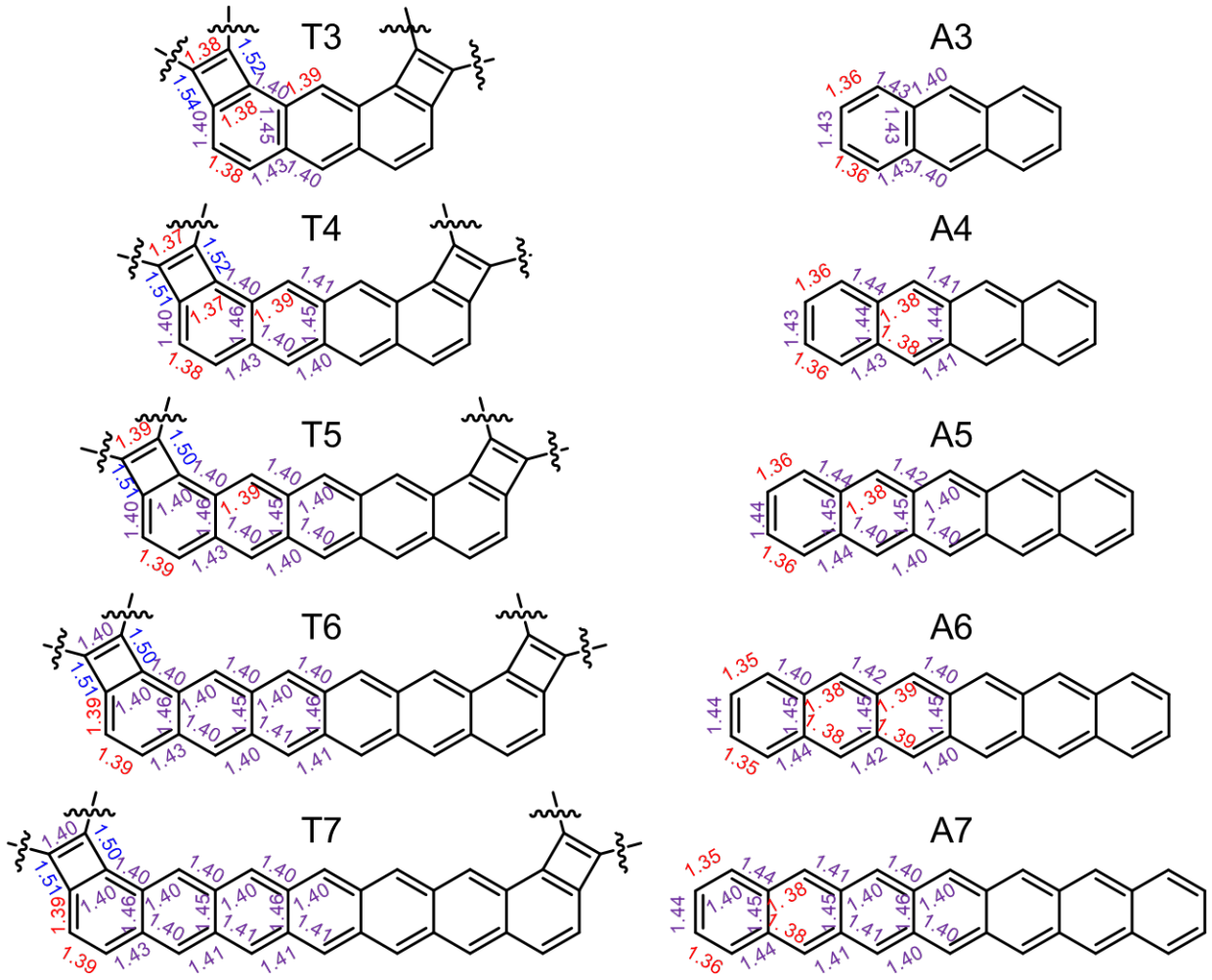

Figure S1. Pertinent bond lengths of the DFT-optimized structures of the Tn and An series. Bond lengths ≥ 1.50 are in blue, bond lengths < 1.40 are in red, while those in between are in purple.

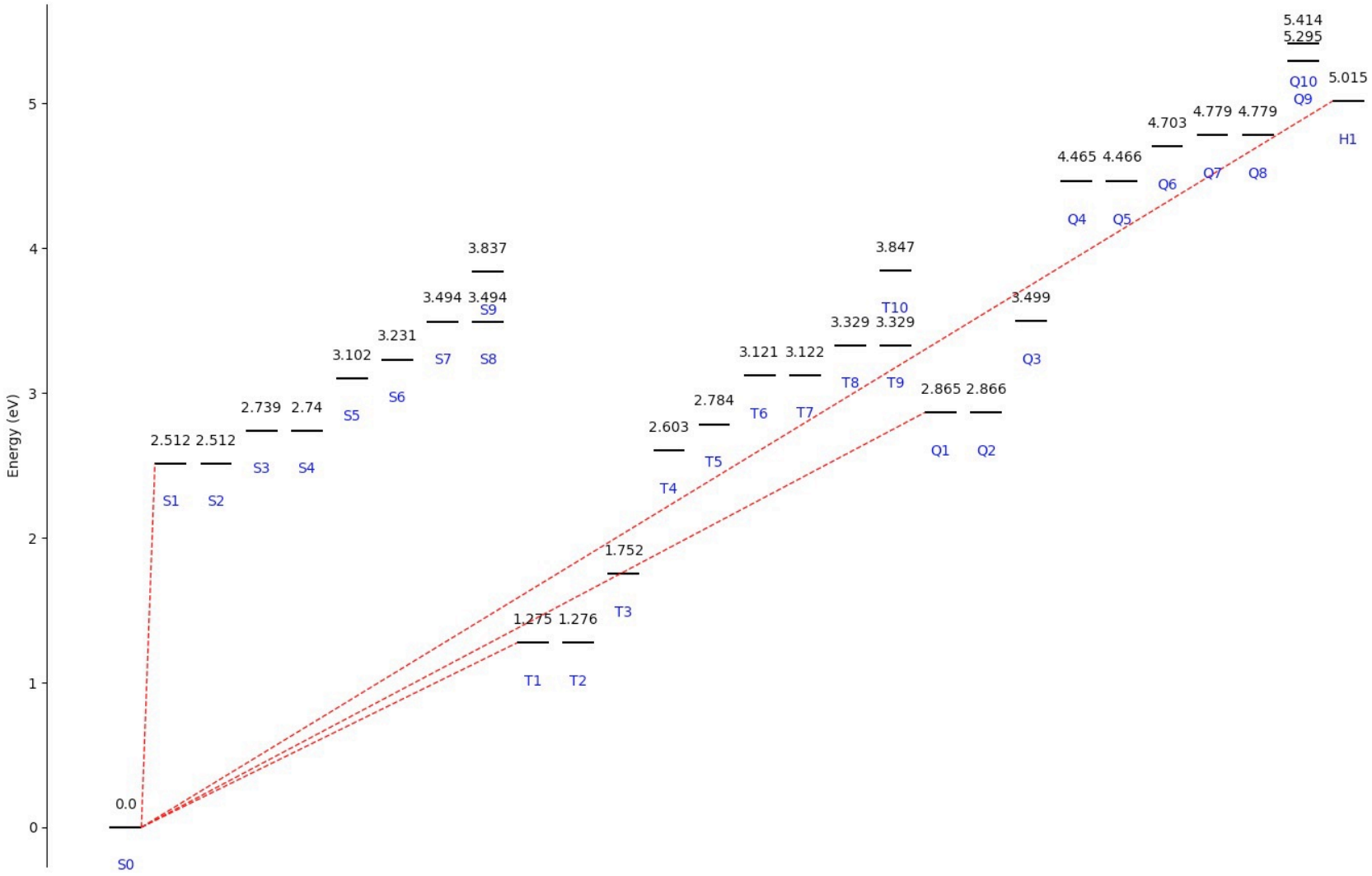

Figure S2. RASCI(h,p)/6-31G(d,p) Computed states with RASCI (10 roots) for **T3**.

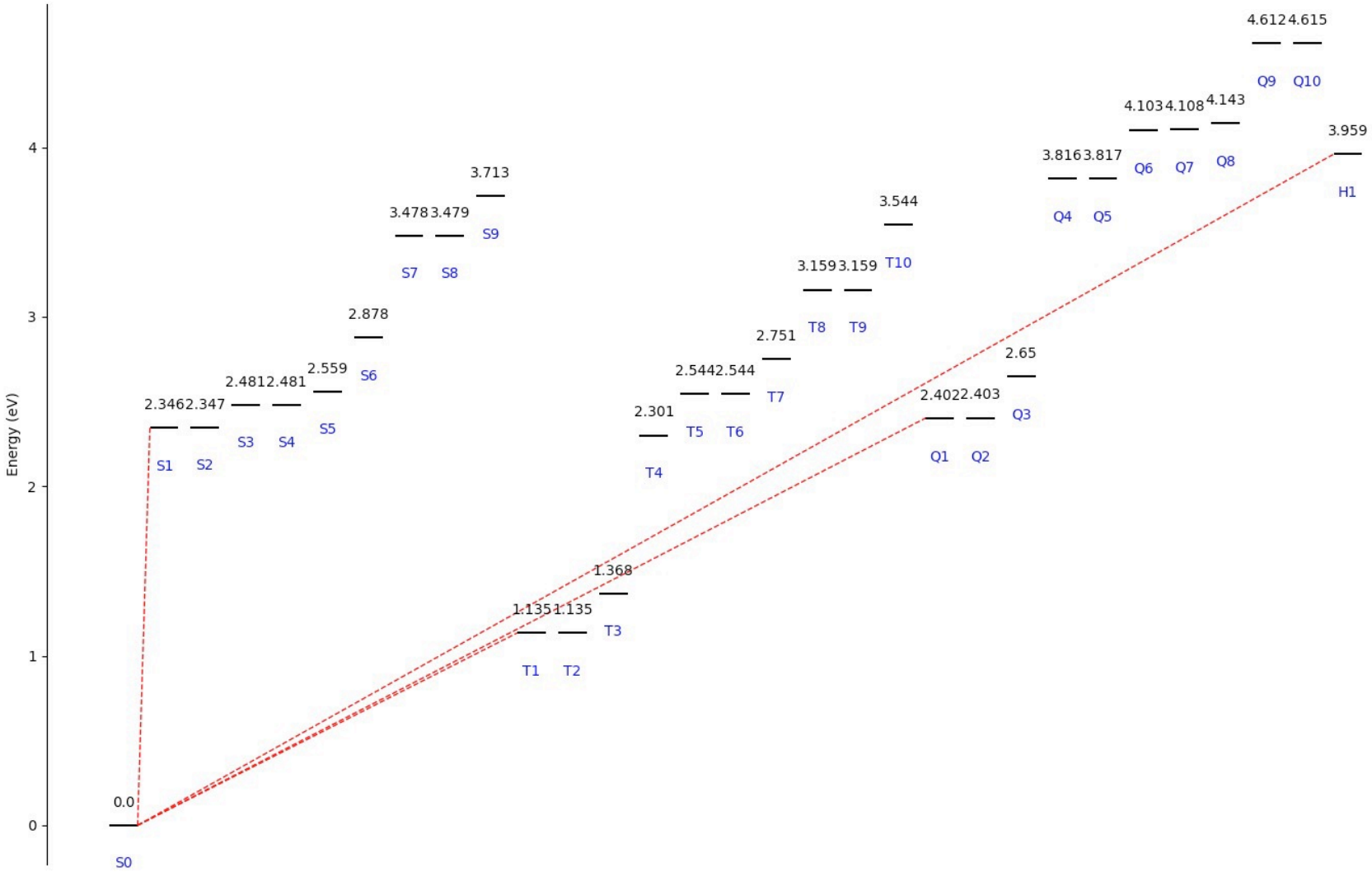

Figure S3. RASCI(h,p)/6-31G(d,p) Computed states with RASCI (10 roots) for **T4**.

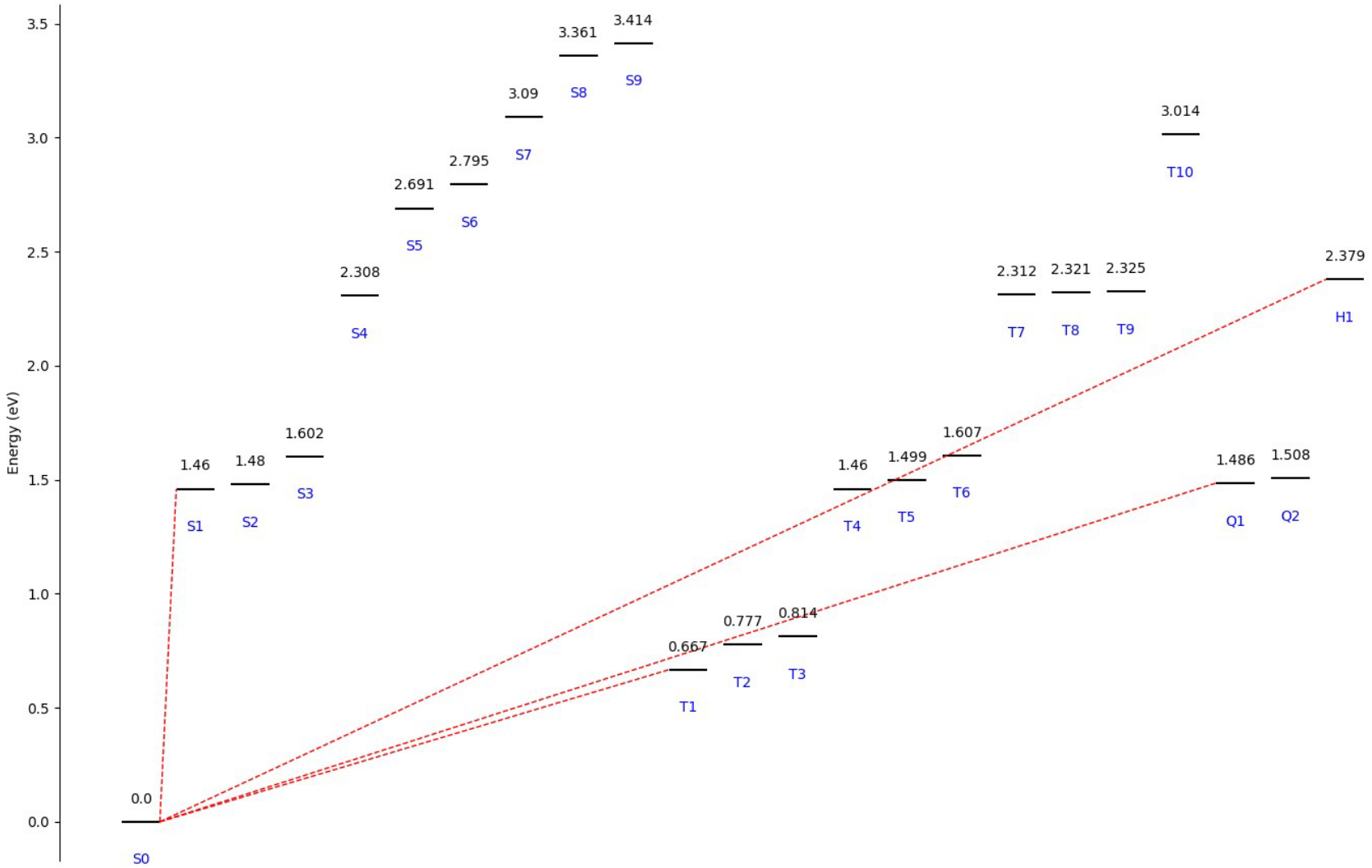

Figure S4. RASCI(h,p)/6-31G(d,p) Computed states with RASCI (10 roots) for **T5**.

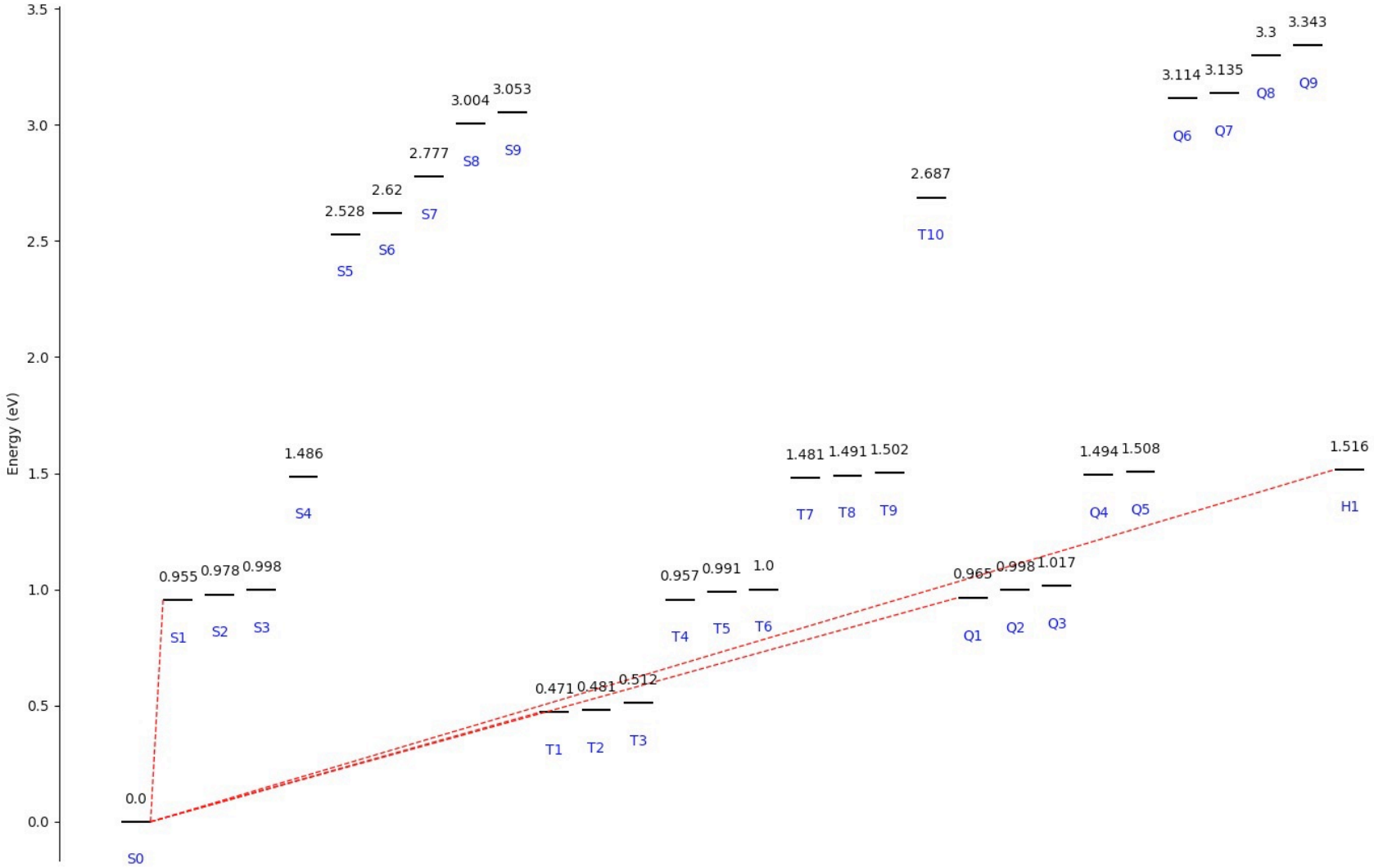

Figure S5. RASCI(h,p)/6-31G(d,p) Computed states with RASCI (10 roots) for **T6**.

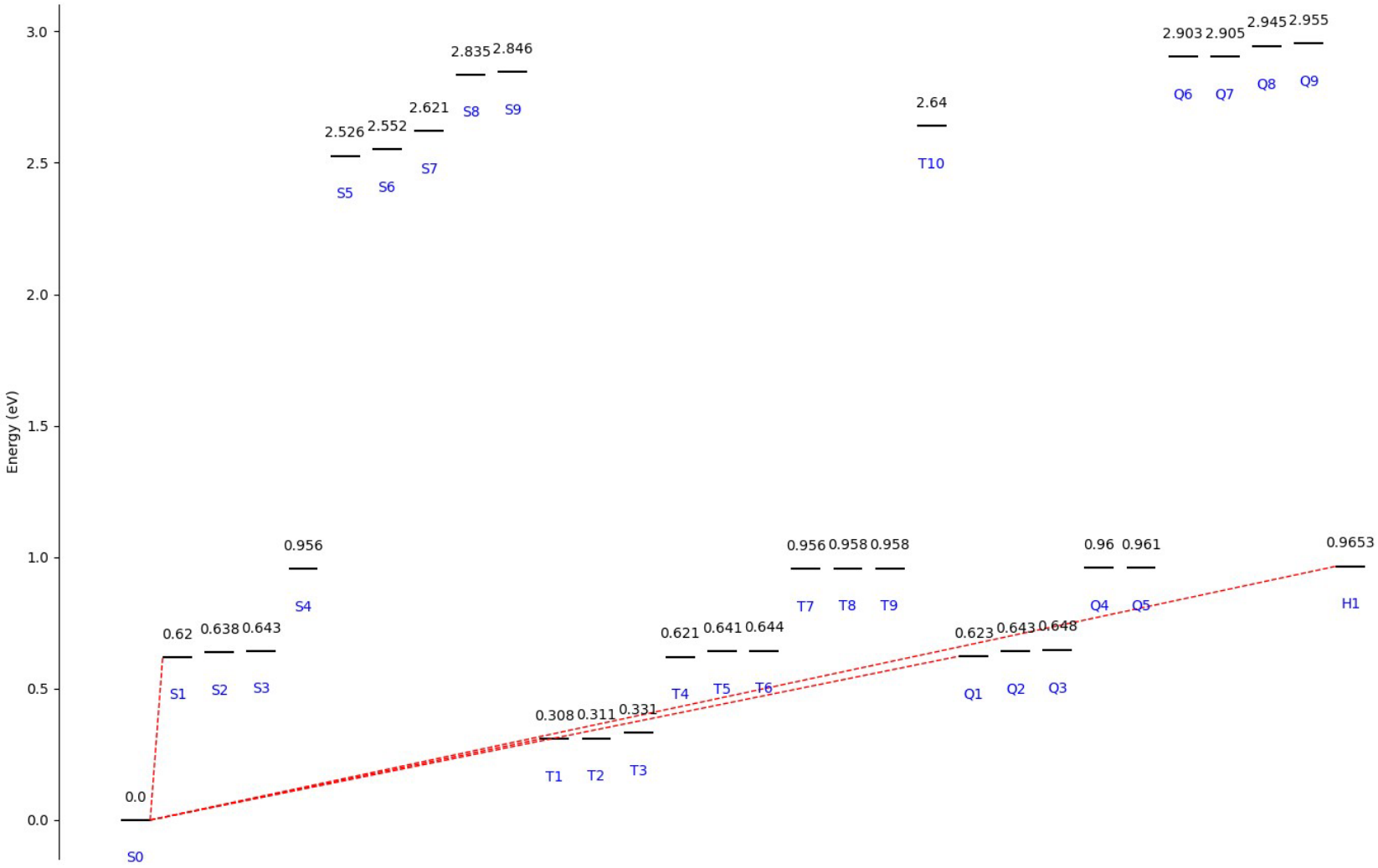

Figure S6. RASCI(h,p)/6-31G(d,p) Computed states with RASCI (10 roots) for **T6**.

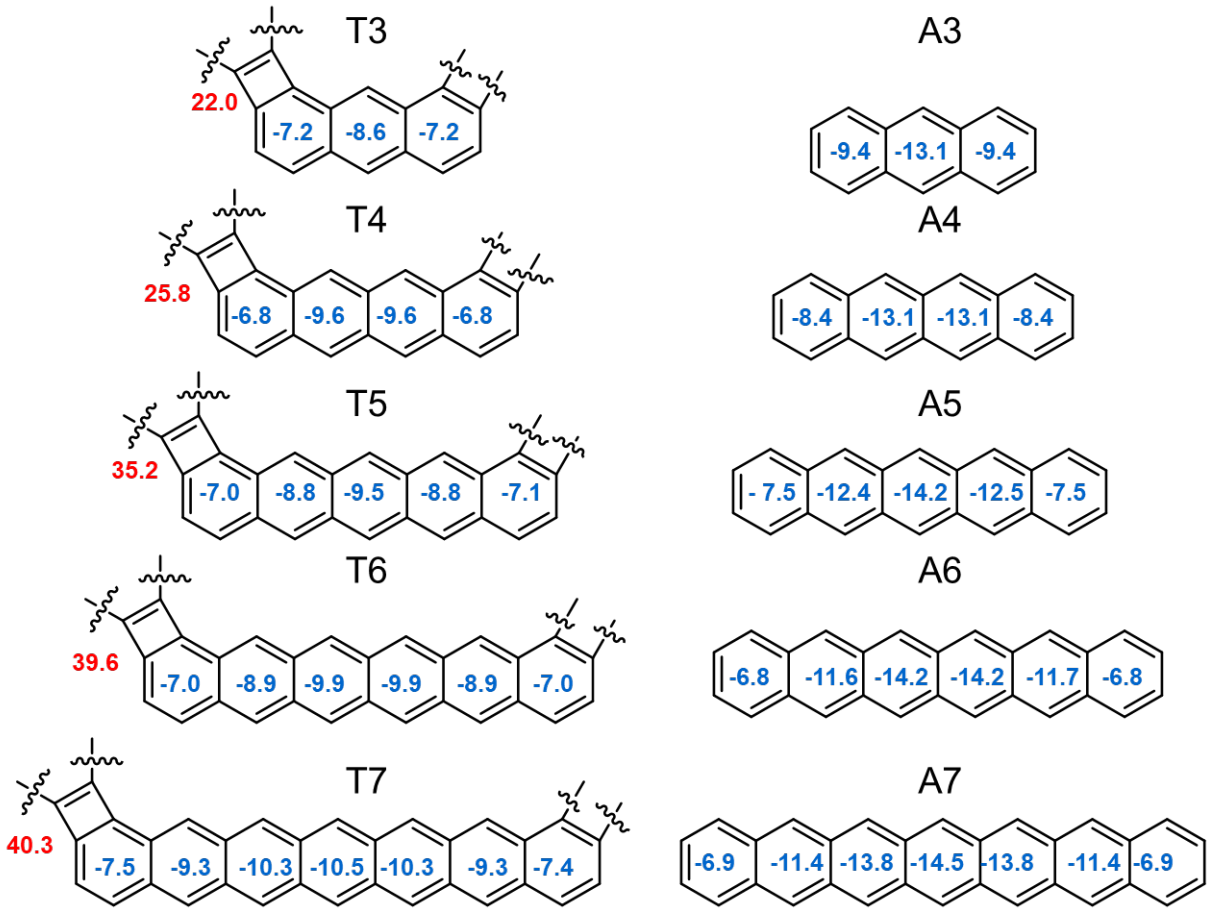

Figure S7. NICS(1) values calculated at the M062x/6-311++g(2d,p) level of theory on the DFT-optimized ground state structures.

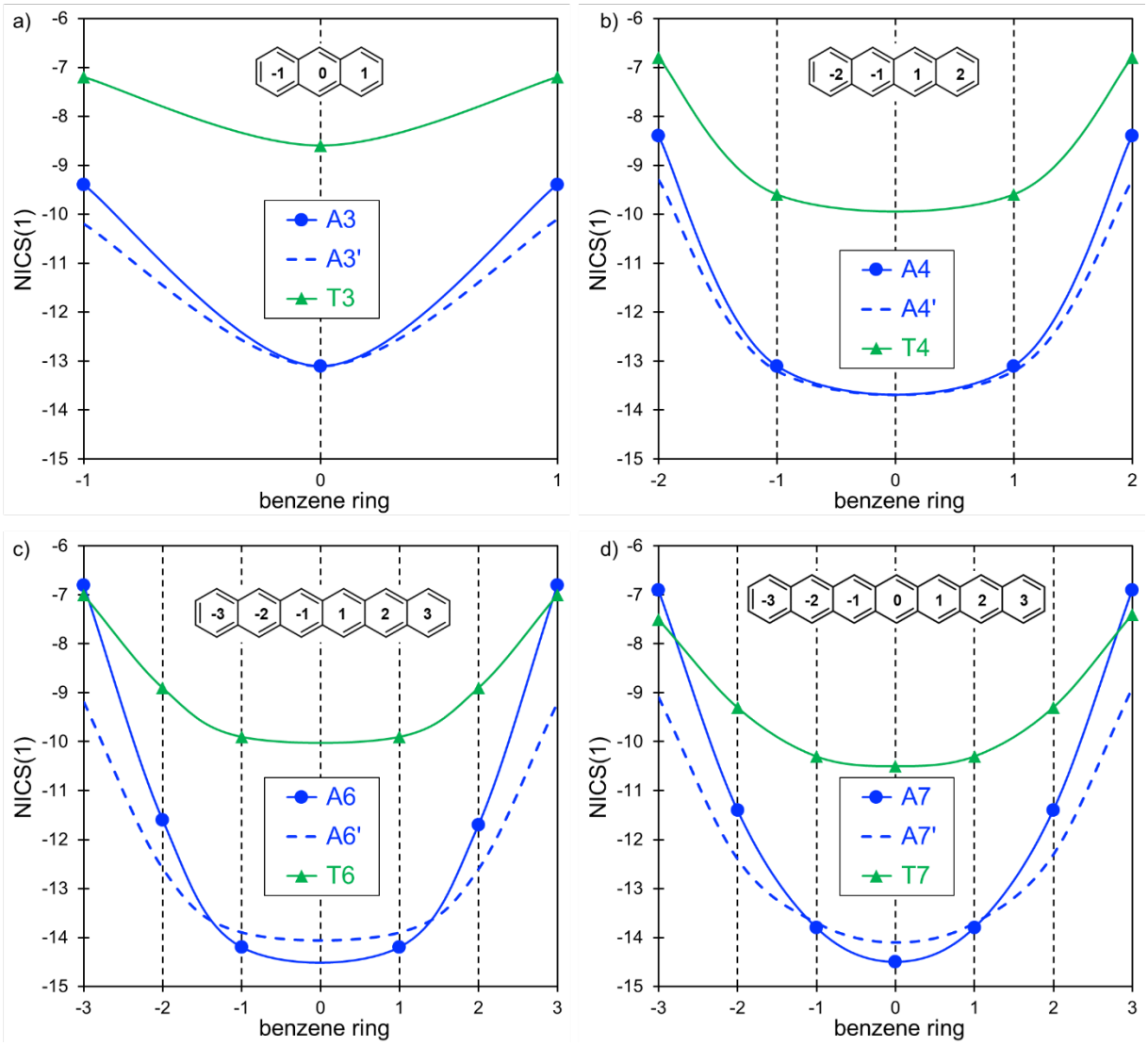

Figure S8. NICS(1) values computed at the M06-2X/6-311+G(d,p) level at the center of the six-member rings in (a) A3, A3', T3; (b) A4, A4', T4; (c) A6, A6', T6 and; (d) A7, A7', T7 molecules.

Cartesian coordinates of optimized Tn series

T3 restricted (S=0)

C	-4.560481	-1.259753	-0.000243
C	-3.193662	-1.101432	-0.000778
C	-2.288741	-2.171552	-0.000597
C	-2.892199	-3.492656	0.000185
C	-4.315955	-3.617729	0.000704
C	-5.164531	-2.525606	0.000548
C	-0.904309	-2.037133	-0.000965
C	-2.045380	-4.608564	0.000532
C	-0.649656	-4.487818	0.000244
C	-0.074941	-3.154032	-0.000520
C	1.325514	-3.107064	-0.000690
C	2.125248	-4.226974	-0.000093
C	1.591885	-5.524033	0.000690
C	0.212626	-5.627415	0.000806
H	-0.466658	-1.050885	-0.001572
H	-4.733282	-4.618844	0.001285
H	-6.238730	-2.660069	0.001003
H	-2.485830	-5.601435	0.001117
H	2.212754	-6.410891	0.001183
H	-0.249560	-6.608613	0.001383
C	3.371060	-3.319547	-0.000138
C	4.769377	-3.209883	0.000499
C	2.550781	-2.214993	-0.000664
C	5.291049	-1.929003	0.000520
H	5.422830	-4.072987	0.000937
H	6.366734	-1.790109	0.000919
C	4.471060	-0.758401	0.000044
C	5.014130	0.532837	0.000251
C	3.025204	-0.896104	-0.000536
C	4.211764	1.681415	0.000025
H	6.094213	0.647733	0.000678
C	2.216752	0.235725	-0.000843
C	2.769320	1.512316	-0.000529
C	4.767383	2.998021	0.000434
H	1.143833	0.121651	-0.001290
C	2.028155	2.701514	-0.000651
C	3.988049	4.140756	0.000411
H	5.848203	3.088567	0.000865
C	2.598064	3.953954	-0.000136
H	4.445446	5.121953	0.000854
C	0.642861	3.316298	-0.000516
C	1.189140	4.579032	0.000024
C	0.395033	5.735245	0.000744
C	-0.975042	5.546456	0.000985
H	0.815737	6.732741	0.001225
H	-1.633254	6.408500	0.001687
C	-0.736457	3.067624	-0.000432
C	-1.578661	4.250925	0.000272

C	-1.312396	1.801582	-0.000904
C	-2.968452	4.075680	0.000409
C	-2.694372	1.641894	-0.000626
H	-0.677298	0.929296	-0.001475
C	-3.561911	2.806628	0.000044
H	-3.607886	4.953696	0.000960
C	-3.353871	0.405584	-0.000909
C	-4.979911	2.629710	0.000487
C	-4.723485	0.272997	-0.000356
C	-5.580086	1.383497	0.000332
H	-5.598465	3.520649	0.001044
H	-6.658537	1.289075	0.000814

T3 urestricted (S=1)

C	-1.676159	-4.430952	-0.000024
C	-0.991100	-3.216282	-0.000376
C	0.390483	-3.118258	-0.000327
C	1.107472	-4.374733	0.000109
C	0.391526	-5.588730	0.000437
C	-1.009061	-5.643956	0.000400
C	1.110241	-1.903840	-0.000584
C	2.530868	-4.328273	0.000266
C	3.235253	-3.138516	0.000084
C	2.484294	-1.886421	-0.000341
C	3.275736	-0.713461	-0.000433
C	4.716220	-0.734717	-0.000089
C	5.426397	-1.933603	0.000310
C	4.680249	-3.104274	0.000363
H	0.563941	-0.974063	-0.000981
H	0.956916	-6.514311	0.000770
H	-1.520500	-6.598228	0.000719
H	3.076975	-5.267103	0.000586
H	6.508518	-1.973130	0.000597
H	5.193766	-4.059411	0.000673
C	4.716482	0.732866	-0.000089
C	5.427154	1.931492	0.000281
C	3.276040	0.712173	-0.000413
C	4.681486	3.102440	0.000317
H	6.509291	1.970565	0.000552
H	5.195371	4.057378	0.000601
C	3.236493	3.137246	0.000054
C	2.532574	4.327285	0.000222
C	2.485052	1.885460	-0.000336
C	1.109210	4.374293	0.000085
H	3.079054	5.265898	0.000516
C	1.111006	1.903407	-0.000532
C	0.391731	3.118101	-0.000298
C	0.393730	5.588584	0.000397
H	0.564344	0.973842	-0.000860
C	-0.989824	3.216670	-0.000359
C	-1.006818	5.644352	0.000388

H	0.959490	6.513938	0.000693
C	-1.674394	4.431594	0.000002
H	-1.517895	6.598818	0.000698
C	-2.301936	2.472650	-0.000347
C	-2.999647	3.660129	-0.000014
C	-4.403943	3.697712	0.000335
C	-5.057630	2.480859	0.000335
H	-4.962402	4.625152	0.000614
H	-6.141997	2.456875	0.000605
C	-2.916625	1.211050	-0.000330
C	-4.366445	1.227488	0.000042
C	-2.232670	0.000435	-0.000558
C	-5.043692	0.000990	0.000174
C	-2.917102	-1.209910	-0.000365
H	-1.154077	0.000222	-0.000863
C	-4.366928	-1.225777	0.000018
H	-6.129822	0.001202	0.000454
C	-2.302910	-2.471753	-0.000446
C	-5.058610	-2.478873	0.000317
C	-3.001094	-3.658957	-0.000078
C	-4.405403	-3.695985	0.000307
H	-6.142968	-2.454462	0.000601
H	-4.964233	-4.623203	0.000602

T3 urestricted (S=2)

C	0.759760	-4.695191	-0.000029
C	0.746980	-3.291506	-0.000387
C	1.893839	-2.517200	-0.000353
C	3.140678	-3.244735	0.000076
C	3.127935	-4.651275	0.000399
C	1.943209	-5.407963	0.000377
C	1.908164	-1.103825	-0.000607
C	4.352979	-2.488250	0.0002370
C	4.370301	-1.104789	0.0000660
C	3.089373	-0.393997	-0.0003560
C	3.185346	1.007178	-0.000452
C	4.456530	1.723650	-0.000066
C	5.657774	1.049389	0.000341
C	5.597769	-0.353026	0.000363
H	0.969326	-0.574191	-0.001011
H	4.081380	-5.168765	0.000722
H	1.982909	-6.489714	0.000693
H	5.295310	-3.028168	0.000562
H	6.617311	1.551637	0.000669
H	6.522739	-0.918525	0.000671
C	3.702504	2.987545	-0.000056
C	3.714476	4.388348	0.000320
C	2.480670	2.254905	-0.000390
C	2.486263	5.023635	0.000354
H	4.631704	4.963813	0.000592
H	2.448420	6.107515	0.000643
C	1.228434	4.319904	0.000073

C	0.000899	4.996283	0.000237
C	1.212240	2.880471	-0.000329
C	-1.226868	4.320340	0.000078
H	0.001086	6.082392	0.000536
C	0.000403	2.198870	-0.000539
C	-1.211183	2.880895	-0.000310
C	-2.484450	5.024531	0.000359
H	0.000214	1.120619	-0.000867
C	-2.479849	2.255792	-0.000373
C	-3.712897	4.389686	0.000331
H	-2.446206	6.108396	0.000639
C	-3.701431	2.988884	-0.000026
H	-4.629904	4.965503	0.000601
C	-3.184978	1.008341	-0.000370
C	-4.455898	1.725262	-0.000027
C	-5.657394	1.051416	0.000339
C	-5.597896	-0.351000	0.000344
H	-6.616742	1.554026	0.000637
H	-6.523076	-0.916157	0.000623
C	-3.089522	-0.392883	-0.000330
C	-4.370695	-1.103216	0.000061
C	-1.908570	-1.103131	-0.000565
C	-4.353871	-2.486682	0.000204
C	-1.894751	-2.516505	-0.000348
H	-0.969533	-0.573852	-0.000912
C	-3.141848	-3.243597	0.000043
H	-5.296403	-3.026248	0.000504
C	-0.748169	-3.291236	-0.000429
C	-3.129616	-4.650149	0.000349
C	-0.761462	-4.694907	-0.000051
C	-1.945176	-5.407258	0.000338
H	-4.083254	-5.167284	0.000651
H	-1.985275	-6.488995	0.000659

T3 urestricted (S=3)

C	4.313915	2.067483	-0.000047
C	2.931294	1.628498	-0.000424
C	1.837046	2.522947	-0.000377
C	2.179688	3.916039	0.000069
C	3.573522	4.317446	0.000384
C	4.635358	3.424761	0.000359
C	0.500140	2.135990	-0.000630
C	1.136769	4.854602	0.000254
C	-0.214488	4.476684	0.000081
C	-0.525905	3.076302	-0.000359
C	-1.903490	2.760471	-0.000412
C	-2.947492	3.767619	-0.000017
C	-2.633062	5.126532	0.000385
C	-1.285291	5.455160	0.000402
H	0.254441	1.086917	-0.001023
H	3.777804	5.382430	0.000702
H	5.655904	3.786748	0.000668

H	1.384391	5.911980	0.000598
H	-3.386886	5.903908	0.000695
H	-0.995721	6.500170	0.000714
C	-3.947367	2.702150	-0.000025
C	-5.283590	2.302048	0.000345
C	-2.876006	1.724149	-0.000401
C	-5.525935	0.936174	0.000347
H	-6.107361	3.004850	0.000642
H	-6.550471	0.580887	0.000633
C	-4.481493	-0.070375	0.000047
C	-4.772854	-1.442915	0.000208
C	-3.103778	0.329293	-0.000357
C	-3.769960	-2.424249	0.000046
H	-5.812398	-1.757129	0.000514
C	-2.100233	-0.635002	-0.000584
C	-2.401560	-1.993706	-0.000347
C	-4.081703	-3.840871	0.000336
H	-1.068836	-0.323210	-0.000914
C	-1.439062	-3.028685	-0.000394
C	-3.123063	-4.843632	0.000336
H	-5.131443	-4.112808	0.000610
C	-1.789024	-4.436372	-0.000015
H	-3.419323	-5.885164	0.000628
C	-0.055237	-3.352525	-0.000369
C	-0.366383	-4.769404	0.000000
C	0.648226	-5.726484	0.000385
C	1.952225	-5.253370	0.000400
H	0.451553	-6.791319	0.000685
H	2.772311	-5.962847	0.000702
C	1.266597	-2.852171	-0.000338
C	2.301540	-3.845577	0.000088
C	1.599991	-1.500980	-0.000602
C	3.635875	-3.411841	0.000246
C	2.927399	-1.082668	-0.000371
H	0.814327	-0.763630	-0.000967
C	3.984368	-2.052724	0.000054
H	4.427629	-4.155151	0.000574
C	3.342670	0.268219	-0.000448
C	5.367121	-1.614614	0.000350
C	4.736836	0.668777	-0.000055
C	5.756419	-0.283125	0.000328
H	6.127373	-2.387868	0.000646
H	6.806575	-0.019076	0.000626

T4 restricted

C	-0.69536	4.30774	-0.00003
C	-0.10889	5.64175	-0.00007
C	-0.96602	6.79232	-0.00018
C	-2.34112	6.69835	-0.00017
H	-0.31523	2.20099	0.00007
C	0.12341	3.19035	0.00003
C	1.27915	5.75458	-0.00006
H	-0.49459	7.76903	-0.00024
H	-2.95744	7.58841	-0.00022
H	1.72943	6.74282	-0.00016
C	1.51881	3.30905	0.00005
C	2.12246	4.62458	-0.00000
C	2.33870	2.17376	0.00012
C	3.52918	4.72210	-0.00001
C	3.71978	2.28167	0.00012
H	1.87462	1.19610	0.00017
C	4.34872	3.59621	0.00004
H	3.98485	5.70786	-0.00006
C	4.61160	1.19542	0.00017
C	5.77993	3.69656	-0.00001
C	5.97651	1.33386	0.00010
C	6.60527	2.59268	0.00001
H	6.21309	4.69083	-0.00008
H	7.68198	2.70558	-0.00005
C	6.12029	-0.20151	0.00011
C	6.97175	-1.32183	-0.00007
C	4.75340	-0.31880	0.00019
C	6.36571	-2.55972	-0.00014
H	8.05071	-1.23294	-0.00015
C	4.07877	-1.55175	0.00012
C	4.94072	-2.72678	-0.00005
H	6.97591	-3.45632	-0.00027
C	2.70171	-1.70196	0.00020
C	4.34431	-3.98516	-0.00013
C	2.10663	-2.96961	0.00009
H	2.06449	-0.82722	0.00035
H	4.97485	-4.86935	-0.00024
C	2.94394	-4.15031	-0.00007
C	2.32492	-5.41720	-0.00016
C	0.71347	-3.11197	0.00013
C	0.94007	-5.56391	-0.00012
H	2.95063	-6.30482	-0.00027
C	0.11626	-4.36186	0.00002
H	0.09883	-2.22121	0.00027
C	0.31142	-6.85354	-0.00020
C	-1.27041	-4.59101	0.00004
C	-1.05720	-7.01635	-0.00016
H	0.95582	-7.72588	-0.00030
C	-1.83295	-5.84233	-0.00003
H	-1.49773	-8.00527	-0.00023
C	-2.10049	4.27561	-0.00006

C	-2.88555	5.40080	-0.00011
C	-3.34104	3.39582	-0.00007
C	-3.83613	2.08041	-0.00001
C	-4.14335	4.50869	-0.00008
C	-5.28900	1.96795	0.00004
C	-3.05225	0.93830	0.00001
C	-5.54794	4.42391	-0.00002
C	-5.85433	0.69529	0.00008
C	-6.09137	3.15731	0.00004
H	-1.97352	1.02531	-0.00003
H	-6.18396	5.30000	-0.00003
H	-6.93587	0.59710	0.00010
H	-7.16905	3.03554	0.00008
C	-5.06665	-0.47428	0.00008
C	-5.62365	-1.76972	0.00009
C	-3.62553	-0.33938	0.00005
C	-4.83194	-2.91536	0.00007
H	-6.70463	-1.87394	0.00010
C	-2.82512	-1.48850	0.00005
C	-5.39956	-4.23308	0.00004
C	-3.38345	-2.75616	0.00007
H	-1.74897	-1.37389	0.00001
C	-4.63038	-5.37674	-0.00000
H	-6.48111	-4.31351	0.00004
C	-2.65279	-3.95686	0.00006
C	-3.23449	-5.19932	0.00000
H	-5.09281	-6.35562	-0.00004

T4 unrestricted (S=0)

C	-0.69536	4.30774	-0.00003
C	-0.10889	5.64175	-0.00007
C	-0.96602	6.79232	-0.00018
C	-2.34112	6.69835	-0.00017
H	-0.31523	2.20099	0.00007
C	0.12341	3.19035	0.00003
C	1.27915	5.75458	-0.00006
H	-0.49459	7.76903	-0.00024
H	-2.95744	7.58841	-0.00022
H	1.72943	6.74282	-0.00016
C	1.51881	3.30905	0.00005
C	2.12246	4.62458	-0.00000
C	2.33870	2.17376	0.00012
C	3.52918	4.72210	-0.00001
C	3.71978	2.28167	0.00012
H	1.87462	1.19610	0.00017
C	4.34872	3.59621	0.00004
H	3.98485	5.70786	-0.00006
C	4.61160	1.19542	0.00017
C	5.77993	3.69656	-0.00001
C	5.97651	1.33386	0.00010
C	6.60527	2.59268	0.00001
H	6.21309	4.69083	-0.00008

H	7.68198	2.70558	-0.00005
C	6.12029	-0.20151	0.00011
C	6.97175	-1.32183	-0.00007
C	4.75340	-0.31880	0.00019
C	6.36571	-2.55972	-0.00014
H	8.05071	-1.23294	-0.00015
C	4.07877	-1.55175	0.00012
C	4.94072	-2.72678	-0.00005
H	6.97591	-3.45632	-0.00027
C	2.70171	-1.70196	0.00020
C	4.34431	-3.98516	-0.00013
C	2.10663	-2.96961	0.00009
H	2.06449	-0.82722	0.00035
H	4.97485	-4.86935	-0.00024
C	2.94394	-4.15031	-0.00007
C	2.32492	-5.41720	-0.00016
C	0.71347	-3.11197	0.00013
C	0.94007	-5.56391	-0.00012
H	2.95063	-6.30482	-0.00027
C	0.11626	-4.36186	0.00002
H	0.09883	-2.22121	0.00027
C	0.31142	-6.85354	-0.00020
C	-1.27041	-4.59101	0.00004
C	-1.05720	-7.01635	-0.00016
H	0.95582	-7.72588	-0.00030
C	-1.83295	-5.84233	-0.00003
H	-1.49773	-8.00527	-0.00023
C	-2.10049	4.27561	-0.00006
C	-2.88555	5.40080	-0.00011
C	-3.34104	3.39582	-0.00007
C	-3.83613	2.08041	-0.00001
C	-4.14335	4.50869	-0.00008
C	-5.28900	1.96795	0.00004
C	-3.05225	0.93830	0.00001
C	-5.54794	4.42391	-0.00002
C	-5.85433	0.69529	0.00008
C	-6.09137	3.15731	0.00004
H	-1.97352	1.02531	-0.00003
H	-6.18396	5.30000	-0.00003
H	-6.93587	0.59710	0.00010
H	-7.16905	3.03554	0.00008
C	-5.06665	-0.47428	0.00008
C	-5.62365	-1.76972	0.00009
C	-3.62553	-0.33938	0.00005
C	-4.83194	-2.91536	0.00007
H	-6.70463	-1.87394	0.00010
C	-2.82512	-1.48850	0.00005
C	-5.39956	-4.23308	0.00004
C	-3.38345	-2.75616	0.00007
H	-1.74897	-1.37389	0.00001
C	-4.63038	-5.37674	-0.00000
H	-6.48111	-4.31351	0.00004
C	-2.65279	-3.95686	0.00006

C	-3.23449	-5.19932	0.00000
H	-5.09281	-6.35562	-0.00004

T4 unrestricted (S=1)

C	3.62528	-2.42836	-0.00001
C	5.08154	-2.45237	-0.00001
C	5.76881	-3.71263	-0.00001
C	5.11003	-4.92246	-0.00001
H	1.86972	-1.20426	-0.00001
C	2.95175	-1.21869	-0.00001
C	5.76384	-1.23866	-0.00000
H	6.85320	-3.69217	-0.00001
H	5.66149	-5.85404	-0.00001
H	6.84982	-1.24219	-0.00000
C	3.64213	-0.00022	0.00000
C	5.08890	-0.00030	0.00000
C	2.95190	1.21834	0.00001
C	5.76399	1.23797	0.00001
C	3.62557	2.42793	0.00001
H	1.86987	1.20404	0.00001
C	5.08184	2.45176	0.00001
H	6.84997	1.24137	0.00001
C	3.00813	3.69181	0.00002
C	5.76926	3.71194	0.00002
C	3.70320	4.87590	0.00002
C	5.11063	4.92185	0.00002
H	6.85364	3.69135	0.00002
H	5.66220	5.85337	0.00002
C	2.37379	5.64808	0.00002
C	1.71139	6.87463	0.00002
C	1.69238	4.44401	0.00002
C	0.32158	6.83071	0.00001
H	2.23352	7.82303	0.00002
C	0.30123	4.34786	0.00001
C	-0.40892	5.61261	0.00001
H	-0.24056	7.75823	0.00001
C	-0.41962	3.14717	0.00001
C	-1.81891	5.58246	0.00001
C	-1.80402	3.13836	0.00000
H	0.11171	2.20432	0.00001
H	-2.36177	6.52306	0.00001
C	-2.53351	4.38756	0.00001
C	-3.96211	4.33443	0.00000
C	-2.52357	1.91790	0.00000
C	-4.65689	3.14401	0.00000
H	-4.51159	5.27112	0.00001
C	-3.89693	1.88944	-0.00000
H	-1.96213	0.99316	-0.00000
C	-6.10112	3.10341	-0.00000
C	-4.68374	0.71694	-0.00001
C	-6.83885	1.92951	-0.00000
H	-6.61906	4.05613	0.00000

C	-6.12023	0.73406	-0.00001
H	-7.92124	1.96089	-0.00001
C	3.00769	-3.69217	-0.00002
C	3.70261	-4.87634	-0.00002
C	1.69184	-4.44421	-0.00001
C	0.30070	-4.34790	-0.00001
C	2.37311	-5.64836	-0.00001
C	-0.40960	-5.61256	-0.00001
C	-0.42000	-3.14712	-0.00000
C	1.71056	-6.87483	-0.00001
C	-1.81958	-5.58224	-0.00001
C	0.32076	-6.83075	-0.00001
H	0.11145	-2.20433	0.00000
H	2.23258	-7.82329	-0.00001
H	-2.36255	-6.52278	-0.00001
H	-0.24149	-7.75821	-0.00001
C	-2.53404	-4.38725	-0.00001
C	-3.96263	-4.33396	-0.00001
C	-1.80440	-3.13814	-0.00001
C	-4.65727	-3.14345	-0.00001
H	-4.51222	-5.27058	-0.00001
C	-2.52381	-1.91760	-0.00000
C	-6.10150	-3.10268	-0.00001
C	-3.89716	-1.88898	-0.00001
H	-1.96225	-0.99292	-0.00000
C	-6.83908	-1.92869	-0.00001
H	-6.61955	-4.05534	-0.00001
C	-4.68383	-0.71637	-0.00001
C	-6.12032	-0.73333	-0.00001
H	-7.92148	-1.95994	-0.00001

T4 unrestricted (S=2)

C	-4.31548	-0.27858	0.00002
C	-5.60021	0.44007	-0.00002
C	-6.82809	-0.30466	-0.00006
C	-6.89372	-1.70549	-0.00006
H	-2.18771	-0.09408	0.00010
C	-3.13348	0.43124	0.00006
C	-5.58075	1.82018	-0.00003
H	-7.75063	0.26501	-0.00008
H	-7.85348	-2.20681	-0.00009
H	-6.52107	2.36330	-0.00006
C	-3.11019	1.84891	0.00006
C	-4.36328	2.57596	0.00000
C	-1.91352	2.53804	0.00009
C	-4.33189	3.96328	-0.00002
C	-1.87647	3.94306	0.00006
H	-0.98612	1.98048	0.00013
C	-3.11617	4.69098	-0.00000
H	-5.26787	4.51407	-0.00007
C	-0.71471	4.70880	0.00008
C	-3.08314	6.10687	-0.00005

C	-0.71386	6.09925	0.00002
C	-1.89379	6.83477	-0.00005
H	-4.02966	6.63645	-0.00010
H	-1.91099	7.91736	-0.00010
C	0.81468	6.08631	0.00002
C	2.00692	6.80237	-0.00007
C	0.79239	4.69637	0.00009
C	3.18378	6.05517	-0.00008
H	2.04189	7.88453	-0.00013
C	1.94154	3.91119	0.00007
C	3.19343	4.63857	-0.00002
H	4.13901	6.56888	-0.00015
C	1.95521	2.50603	0.00013
C	4.39672	3.89123	-0.00005
C	3.14043	1.79712	0.00008
H	1.01869	1.96397	0.00021
H	5.34173	4.42636	-0.00012
C	4.40517	2.50335	-0.00001
C	5.60999	1.72766	-0.00006
C	3.14028	0.37921	0.00011
C	5.60646	0.34763	-0.00004
H	6.55917	2.25514	-0.00012
C	4.31020	-0.34962	0.00004
H	2.18593	-0.13041	0.00019
C	6.82227	-0.41759	-0.00009
C	4.39284	-1.74792	0.00004
C	6.86475	-1.81868	-0.00008
H	7.75401	0.13688	-0.00015
C	5.65169	-2.47459	-0.00001
H	7.81603	-2.33592	-0.00013
C	-4.42128	-1.67473	-0.00000
C	-5.69202	-2.38083	-0.00003
C	-3.72384	-2.93468	-0.00001
C	-2.45791	-3.56839	0.00001
C	-4.94812	-3.65142	-0.00003
C	-2.49439	-5.01995	-0.00000
C	-1.24543	-2.90793	0.00002
C	-4.98220	-5.05473	-0.00004
C	-1.29017	-5.71223	0.00000
C	-3.76628	-5.70538	-0.00002
H	-1.21883	-1.82644	0.00002
H	-5.90872	-5.61488	-0.00005
H	-1.30279	-6.79803	-0.00001
H	-3.74191	-6.78966	-0.00002
C	-0.04188	-5.04774	0.00001
C	1.19579	-5.73262	0.00001
C	-0.03012	-3.61052	0.00002
C	2.41092	-5.06027	0.00001
H	1.19063	-6.81848	-0.00001
C	1.19694	-2.92793	0.00003
C	3.67154	-5.76658	-0.00001
C	2.39822	-3.60806	0.00003
H	1.18796	-1.84615	0.00004

C	4.89821	-5.13608	-0.00003
H	3.62921	-6.85030	-0.00003
C	3.67459	-2.99539	0.00004
C	4.88745	-3.73265	-0.00000
H	5.81521	-5.71171	-0.00005

T4 unrestricted (S=3)

C	3.70069	-2.25028	0.00001
C	4.32674	-3.55876	-0.00000
C	5.77445	-3.66415	-0.00001
C	6.62534	-2.57226	-0.00001
H	1.85577	-1.17091	0.00001
C	2.32465	-2.14578	0.00001
C	3.51178	-4.68080	-0.00000
H	6.19354	-4.66420	-0.00001
H	7.69902	-2.71363	-0.00001
H	3.96711	-5.66675	-0.00001
C	1.50225	-3.28598	0.00001
C	2.09664	-4.58662	0.00000
C	0.10193	-3.16159	0.00001
C	1.24164	-5.71838	-0.00000
C	-0.71960	-4.27040	0.00000
H	-0.32831	-2.16903	0.00001
C	-0.13997	-5.60025	-0.00000
H	1.68911	-6.70791	-0.00001
C	-2.13502	-4.22799	0.00000
C	-1.00769	-6.76386	-0.00001
C	-2.95755	-5.41664	-0.00000
C	-2.39023	-6.69276	-0.00001
H	-0.52577	-7.73520	-0.00001
H	-2.98589	-7.59719	-0.00001
C	-4.14829	-4.56929	-0.00000
C	-5.53998	-4.45179	-0.00000
C	-3.29514	-3.40277	0.00000
C	-6.06044	-3.16906	-0.00000
H	-6.19903	-5.31111	-0.00001
C	-3.79943	-2.07956	0.00000
C	-5.24561	-1.96782	-0.00000
H	-7.13609	-3.03227	-0.00001
C	-3.02105	-0.94004	0.00000
C	-5.80999	-0.70102	-0.00000
C	-3.59743	0.34214	0.00000
H	-1.94233	-1.02137	0.00001
H	-6.89153	-0.60263	-0.00000
C	-5.02096	0.47758	0.00000
C	-5.57354	1.78406	-0.00000
C	-2.78954	1.49272	0.00001
C	-4.78043	2.92154	0.00000
H	-6.65424	1.89126	-0.00000
C	-3.33893	2.75857	0.00000
H	-1.71487	1.36898	0.00001
C	-5.35405	4.25495	-0.00000

C	-2.59425	3.96296	0.00000
C	-4.60096	5.41662	-0.00000
H	-6.43620	4.32352	-0.00001
C	-3.21220	5.26978	-0.00000
H	-5.08634	6.38471	-0.00001
C	4.59470	-1.15215	0.00001
C	6.03154	-1.30799	0.00000
C	4.72947	0.26510	0.00001
C	4.05856	1.51208	0.00001
C	6.17012	0.14695	0.00000
C	4.92026	2.67909	-0.00000
C	2.68763	1.66905	0.00001
C	6.99162	1.27647	-0.00001
C	4.33165	3.93462	-0.00000
C	6.36189	2.50933	-0.00001
H	2.04318	0.80021	0.00002
H	8.07271	1.21280	-0.00001
H	4.96477	4.81698	-0.00001
H	6.96209	3.41238	-0.00001
C	2.92394	4.10915	0.00000
C	2.29776	5.38174	-0.00000
C	2.09498	2.94399	0.00001
C	0.91856	5.52622	-0.00000
H	2.92374	6.26917	-0.00001
C	0.69641	3.08583	0.00001
C	0.28587	6.83261	-0.00001
C	0.09869	4.32965	0.00001
H	0.08674	2.19224	0.00002
C	-1.08506	7.02345	-0.00001
H	0.94241	7.69558	-0.00001
C	-1.29947	4.55483	0.00000
C	-1.88292	5.87700	-0.00000
H	-1.49968	8.02390	-0.00001

T5 restricted

C	0.85869	-3.57997	-0.00235
C	-0.16666	-4.52467	-0.00140
C	0.16472	-5.93748	0.00020
C	1.51479	-6.31360	0.00077
C	2.54714	-5.36570	-0.00002
C	-1.51633	-4.13338	-0.00180
C	-0.89160	-6.87915	0.00127
C	-2.22445	-6.49278	0.00098
C	-2.53657	-5.06586	-0.00058
C	-3.91044	-4.75979	-0.00056
C	-4.89835	-5.70905	0.00086
C	-4.62062	-7.09110	0.00237
C	-3.29369	-7.45385	0.00236
H	-1.75111	-3.07673	-0.00302
H	0.60531	-2.52449	-0.00353
H	1.76832	-7.36939	0.00199
H	-0.64605	-7.93696	0.00245

H	-5.40142	-7.84101	0.00351
H	-3.02267	-8.50394	0.00349
C	2.20128	-3.95643	-0.00163
C	3.22639	-2.99532	-0.00225
C	4.55885	-3.36334	-0.00122
H	2.95610	-1.94721	-0.00344
C	3.91570	-5.72553	0.00086
C	5.64443	-2.46735	-0.00131
C	4.92818	-4.77647	0.00038
H	4.17708	-6.77955	0.00207
C	6.95551	-2.86505	0.00016
C	6.31695	-5.14790	0.00169
C	7.33495	-4.22261	0.00168
H	6.55187	-6.20665	0.00286
H	8.37101	-4.53660	0.00284
C	-4.95908	-3.65435	-0.00066
C	-5.19241	-2.26624	-0.00088
C	-5.95900	-4.59093	0.00068
C	-4.20748	-1.29630	-0.00185
C	-6.60089	-1.87961	0.00025
C	-7.32447	-4.24083	0.00172
H	-3.16465	-1.58629	-0.00267
C	-6.91664	-0.52832	0.00033
C	-7.61688	-2.89667	0.00142
H	-8.11433	-4.98119	0.00277
H	-7.96014	-0.22765	0.00119
H	-8.65128	-2.57084	0.00221
C	-4.52733	0.07200	-0.00159
C	-5.92072	0.47704	-0.00044
C	-3.53003	1.04646	-0.00223
C	-6.22545	1.84506	0.00003
C	-3.83549	2.40675	-0.00161
H	-2.48927	0.73811	-0.00307
C	-5.22470	2.82619	-0.00044
H	-7.26654	2.15344	0.00089
C	-2.82181	3.37992	-0.00192
C	-5.51199	4.21191	0.00037
C	-3.11921	4.72966	-0.00098
H	-1.78932	3.05495	-0.00276
C	-4.51097	5.17296	0.00024
H	-6.55085	4.52821	0.00126
C	-2.16706	5.76633	-0.00085
C	-4.80843	6.57953	0.00148
C	-2.49499	7.09650	0.00059
H	-5.85329	6.87009	0.00233
C	-3.83066	7.54712	0.00177
H	-4.08956	8.59830	0.00290
C	7.39359	-1.38748	0.00014
C	8.45158	-0.45589	0.00175
C	6.07761	-1.00655	-0.00132
C	8.10234	0.87466	0.00182
H	9.49139	-0.75724	0.00294
C	5.65587	0.33631	-0.00124

C	6.73548	1.32011	0.00047
H	8.87627	1.63438	0.00304
C	4.33814	0.75350	-0.00242
C	6.40353	2.66755	0.00097
C	4.00213	2.11789	-0.00176
H	3.54056	0.02173	-0.00376
C	5.05987	3.11133	0.00003
H	7.19677	3.40920	0.00227
C	2.67119	2.53347	-0.00259
C	4.71045	4.46862	0.00093
H	1.88392	1.78617	-0.00390
H	5.49803	5.21607	0.00229
C	2.32592	3.88427	-0.00157
C	3.37339	4.88854	0.00024
C	0.98094	4.29157	-0.00206
C	3.00066	6.25375	0.00138
C	0.63350	5.62941	-0.00071
H	0.20840	3.53343	-0.00346
C	1.67263	6.65595	0.00104
H	3.78286	7.00704	0.00266
C	-0.68529	6.12158	-0.00072
C	1.29988	8.04447	0.00250
H	2.09932	8.77730	0.00376
C	-0.01032	8.46334	0.00246
H	-0.25654	9.51755	0.00368
C	-0.99634	7.45575	0.00077

T5 unrestricted (S=0)

C	0.02209	-3.66852	-0.00123
C	-1.19522	-4.35521	-0.00083
C	-1.19396	-5.80740	-0.00011
C	0.03903	-6.47972	0.00017
C	1.26384	-5.79259	-0.00014
C	-2.41437	-3.66738	-0.00101
C	-2.43274	-6.48157	0.00036
C	-3.65265	-5.80124	0.00027
C	-3.63250	-4.34268	-0.00043
C	-4.88974	-3.73199	-0.00035
C	-6.08974	-4.44381	0.00041
C	-6.12685	-5.83812	0.00109
C	-4.90202	-6.49212	0.00096
H	-2.40091	-2.58517	-0.00154
H	0.01552	-2.58311	-0.00177
H	0.04560	-7.56539	0.00071
H	-2.43539	-7.56738	0.00089
H	-7.05274	-6.39925	0.00169
H	-4.87608	-7.57627	0.00146
C	1.24757	-4.34049	-0.00086
C	2.45837	-3.63804	-0.00106
C	3.68454	-4.29863	-0.00051
H	2.43187	-2.55608	-0.00160
C	2.51064	-6.45180	0.00032

C	4.93436	-3.67288	-0.00045
C	3.72228	-5.75685	0.00020
H	2.52639	-7.53751	0.00085
C	6.14283	-4.37020	0.00031
C	4.97988	-6.43267	0.00088
C	6.19672	-5.76393	0.00099
H	4.96702	-7.51706	0.00139
H	7.12927	-6.31393	0.00161
C	-5.64952	-2.43828	-0.00032
C	-5.56440	-1.03795	-0.00039
C	-6.85378	-3.13300	0.00038
C	-4.38347	-0.31176	-0.00098
C	-6.84883	-0.34150	0.00031
C	-8.09370	-2.48096	0.00102
H	-3.43301	-0.82936	-0.00155
C	-6.84943	1.04833	0.00044
C	-8.06682	-1.09858	0.00096
H	-9.03471	-3.01630	0.00161
H	-7.79780	1.57711	0.00098
H	-8.99929	-0.54487	0.00147
C	-4.38445	1.09421	-0.00080
C	-5.65142	1.80509	-0.00005
C	-3.19390	1.81518	-0.00122
C	-5.63927	3.20284	0.00025
C	-3.18025	3.21612	-0.00084
H	-2.25003	1.27921	-0.00178
C	-4.43785	3.93874	-0.00009
H	-6.58317	3.73933	0.00081
C	-1.97649	3.92805	-0.00106
C	-4.40656	5.34599	0.00036
C	-1.95673	5.31797	-0.00051
H	-1.04472	3.37719	-0.00163
C	-3.20816	6.06234	0.00021
H	-5.34630	5.89008	0.00092
C	-0.79669	6.10622	-0.00047
C	-3.18236	7.49298	0.00088
C	-0.81359	7.48244	0.00026
H	-4.13432	8.01255	0.00140
C	-2.00750	8.21937	0.00095
H	-2.02466	9.30184	0.00154
C	6.89107	-3.05027	0.00033
C	8.12307	-2.38333	0.00107
C	5.67858	-2.37013	-0.00042
C	8.07954	-1.00137	0.00104
H	9.07041	-2.90738	0.00169
C	5.57664	-0.97093	-0.00045
C	6.85254	-0.25897	0.00034
H	9.00529	-0.43652	0.00162
C	4.38704	-0.25910	-0.00107
C	6.83631	1.13076	0.00051
C	4.37098	1.14677	-0.00084
H	3.44289	-0.78813	-0.00172
C	5.62923	1.87300	-0.00000

H	7.77823	1.67093	0.00112
C	3.17179	1.85328	-0.00128
C	5.60015	3.27048	0.00034
H	2.23446	1.30595	-0.00191
H	6.53751	3.81830	0.00097
C	3.14118	3.25395	-0.00084
C	4.38993	3.99176	-0.00002
C	1.92893	3.95137	-0.00109
C	4.34171	5.39852	0.00048
C	1.89245	5.34096	-0.00048
H	1.00385	3.38936	-0.00173
C	3.13482	6.10038	0.00031
H	5.27488	5.95381	0.00109
C	0.72303	6.11531	-0.00046
C	3.09190	7.53062	0.00100
H	4.03757	8.06155	0.00158
C	1.90844	8.24284	0.00104
H	1.91261	9.32544	0.00165
C	0.72342	7.49163	0.00028

T5 unrestricted (S=1)

C	3.67317	-0.00001	0.00002
C	4.35252	-1.22124	0.00001
C	5.80495	-1.22882	0.00000
C	6.48505	-0.00001	-0.00000
C	5.80496	1.22880	0.00000
C	3.65755	-2.43671	0.00002
C	6.47183	-2.47155	-0.00001
C	5.78374	-3.68682	-0.00001
C	4.32589	-3.65757	0.00001
C	3.70729	-4.91273	0.00000
C	4.40722	-6.11095	-0.00001
C	5.80363	-6.15924	-0.00002
C	6.46654	-4.94163	-0.00002
H	2.57546	-2.41705	0.00003
H	2.58773	-0.00000	0.00003
H	7.57074	-0.00001	-0.00001
H	7.55763	-2.48078	-0.00002
H	6.35667	-7.08995	-0.00003
H	7.55088	-4.92344	-0.00003
C	4.35253	1.22123	0.00002
C	3.65756	2.43670	0.00002
C	4.32590	3.65756	0.00001
H	2.57547	2.41705	0.00003
C	6.47183	2.47153	-0.00001
C	3.70731	4.91272	0.00001
C	5.78374	3.68681	-0.00000
H	7.55764	2.48076	-0.00002
C	4.40724	6.11094	-0.00001
C	6.46655	4.94161	-0.00002
C	5.80365	6.15922	-0.00002
H	7.55089	4.92342	-0.00003
H	6.35669	7.08993	-0.00003

C	2.40114	-5.66650	0.00000
C	1.00253	-5.57175	0.00001
C	3.08269	-6.87102	-0.00001
C	0.28415	-4.38037	0.00002
C	0.29633	-6.84317	-0.00000
C	2.42052	-8.10391	-0.00002
H	0.81087	-3.43490	0.00003
C	-1.10387	-6.82471	-0.00001
C	1.03637	-8.06448	-0.00002
H	2.94710	-9.04983	-0.00003
H	-1.64199	-7.76797	-0.00002
H	0.47508	-8.99250	-0.00002
C	-1.11198	-4.37362	0.00002
C	-1.83365	-5.62777	0.00000
C	-1.83133	-3.16700	0.00002
C	-3.25211	-5.58999	-0.00000
C	-3.21670	-3.14571	0.00002
H	-1.28488	-2.22910	0.00003
C	-3.95377	-4.39603	0.00000
H	-3.79820	-6.52855	-0.00001
C	-3.92717	-1.92560	0.00002
C	-5.38725	-4.33320	-0.00001
C	-5.30774	-1.88936	0.00001
H	-3.36279	-1.00257	0.00003
C	-6.07107	-3.14292	-0.00000
H	-5.94098	-5.26743	-0.00002
C	-6.08553	-0.72401	0.00001
C	-7.52217	-3.09574	-0.00002
C	-7.52053	-0.72644	-0.00001
H	-8.04152	-4.04791	-0.00003
C	-8.25086	-1.92759	-0.00002
H	-9.33339	-1.95180	-0.00003
C	3.08270	6.87101	-0.00001
C	2.42054	8.10390	-0.00002
C	2.40115	5.66650	0.00001
C	1.03639	8.06448	-0.00002
H	2.94712	9.04982	-0.00003
C	1.00254	5.57175	0.00001
C	0.29635	6.84317	-0.00001
H	0.47510	8.99250	-0.00003
C	0.28416	4.38037	0.00002
C	-1.10385	6.82471	-0.00001
C	-1.11197	4.37362	0.00002
H	0.81088	3.43489	0.00003
C	-1.83363	5.62777	0.00000
H	-1.64197	7.76797	-0.00002
C	-1.83132	3.16700	0.00003
C	-3.25209	5.59000	-0.00001
H	-1.28487	2.22911	0.00004
H	-3.79819	6.52856	-0.00002
C	-3.21669	3.14572	0.00002
C	-3.95376	4.39604	0.00000
C	-3.92716	1.92561	0.00002

C	-5.38724	4.33321	-0.00001
C	-5.30773	1.88937	0.00001
H	-3.36278	1.00258	0.00003
C	-6.07106	3.14294	-0.00001
H	-5.94097	5.26745	-0.00002
C	-6.08553	0.72403	0.00001
C	-7.52216	3.09576	-0.00002
H	-8.04151	4.04793	-0.00003
C	-8.25086	1.92761	-0.00002
H	-9.33338	1.95182	-0.00003
C	-7.52053	0.72646	-0.00001

T5 unrestricted (S=2)

C	-0.00338	3.66342	-0.00008
C	1.22847	4.34134	-0.00006
C	1.23470	5.80473	-0.00003
C	-0.00595	6.47976	-0.00002
C	-1.24538	5.80247	-0.00003
C	2.42582	3.65267	-0.00007
C	2.45875	6.46603	0.00000
C	3.70352	5.77667	0.00001
C	3.67515	4.32284	-0.00003
C	4.90770	3.70835	-0.00001
C	6.12905	4.41583	0.00005
C	6.17533	5.78889	0.00008
C	4.93110	6.45451	0.00006
H	2.40669	2.57046	-0.00010
H	-0.00240	2.57809	-0.00011
H	-0.00694	7.56530	0.00000
H	2.46944	7.55185	0.00003
H	7.09994	6.35198	0.00013
H	4.91435	7.53903	0.00009
C	-1.23647	4.33909	-0.00006
C	-2.43255	3.64822	-0.00006
C	-3.68310	4.31611	-0.00002
H	-2.41145	2.56605	-0.00008
C	-2.47064	6.46153	-0.00000
C	-4.91451	3.69934	0.00001
C	-3.71414	5.76988	0.00001
H	-2.48331	7.54732	0.00002
C	-6.13716	4.40457	0.00005
C	-4.94297	6.44545	0.00004
C	-6.18597	5.77754	0.00007
H	-4.92821	7.53001	0.00006
H	-7.11161	6.33893	0.00010
C	5.66831	2.41200	-0.00001
C	5.57338	1.00839	-0.00002
C	6.87038	3.09063	0.00005
C	4.38406	0.29267	-0.00008
C	6.84384	0.30347	0.00003
C	8.10962	2.42444	0.00008
H	3.43880	0.81968	-0.00013

C	6.82951	-1.09202	0.00004
C	8.06990	1.04723	0.00008
H	9.05432	2.95302	0.00012
H	7.77297	-1.62974	0.00008
H	8.99678	0.48384	0.00011
C	4.37749	-1.10458	-0.00007
C	5.63044	-1.82509	-0.00000
C	3.17051	-1.82541	-0.00012
C	5.59636	-3.24040	0.00002
C	3.15182	-3.20795	-0.00008
H	2.23236	-1.27934	-0.00017
C	4.40125	-3.94468	-0.00001
H	6.53531	-3.78571	0.00008
C	1.92893	-3.92372	-0.00011
C	4.34154	-5.37494	0.00003
C	1.89599	-5.29851	-0.00005
H	1.00568	-3.35953	-0.00017
C	3.15008	-6.06288	0.00002
H	5.27619	-5.92777	0.00009
C	0.72498	-6.08276	-0.00004
C	3.10687	-7.50830	0.00008
C	0.73892	-7.51762	0.00003
H	4.05910	-8.02717	0.00013
C	1.93380	-8.24194	0.00008
H	1.96081	-9.32439	0.00013
C	-6.87604	3.07800	0.00006
C	-8.11405	2.40954	0.00008
C	-5.67272	2.40158	0.00002
C	-8.07180	1.03240	0.00006
H	-9.05973	2.93638	0.00010
C	-5.57520	0.99815	-0.00001
C	-6.84437	0.29091	0.00003
H	-8.99763	0.46730	0.00008
C	-4.38457	0.28460	-0.00005
C	-6.82749	-1.10456	0.00003
C	-4.37545	-1.11263	-0.00006
H	-3.44028	0.81334	-0.00009
C	-5.62707	-1.83544	-0.00001
H	-7.76996	-1.64401	0.00006
C	-3.16715	-1.83125	-0.00009
C	-5.59040	-3.25068	0.00001
H	-2.23001	-1.28346	-0.00013
H	-6.52835	-3.79772	0.00005
C	-3.14593	-3.21375	-0.00007
C	-4.39401	-3.95277	-0.00002
C	-1.92171	-3.92726	-0.00009
C	-4.33166	-5.38293	0.00002
C	-1.88625	-5.30200	-0.00004
H	-0.99951	-3.36137	-0.00014
C	-3.13893	-6.06867	0.00001
H	-5.26528	-5.93748	0.00006
C	-0.71379	-6.08408	-0.00003
C	-3.09305	-7.51401	0.00006

H	-4.04432	-8.03463	0.00010
C	-1.91864	-8.24549	0.00007
H	-1.94365	-9.32798	0.00012
C	-0.72509	-7.51897	0.00003

T5 unrestricted (S=3)

C	-3.40303	1.31370	-0.00078
C	-3.59962	2.69303	-0.00051
C	-4.94113	3.22058	-0.00001
C	-6.01742	2.32325	0.00020
C	-5.82355	0.93534	-0.00001
C	-2.50531	3.58491	-0.00064
C	-5.10954	4.63534	0.00029
C	-4.03738	5.50684	0.00020
C	-2.68678	4.95072	-0.00025
C	-1.64912	5.90778	-0.00019
C	-1.88759	7.32702	0.00026
C	-3.17869	7.85295	0.00063
C	-4.22245	6.94085	0.00058
H	-1.50564	3.17130	-0.00101
H	-2.39040	0.92260	-0.00114
H	-7.03028	2.71444	0.00059
H	-6.11913	5.03518	0.00065
H	-3.37750	8.91729	0.00095
H	-5.24446	7.30347	0.00087
C	-4.47561	0.42445	-0.00051
C	-4.26470	-0.97142	-0.00063
C	-5.31696	-1.86080	-0.00024
H	-3.24653	-1.33717	-0.00099
C	-6.89909	0.00093	0.00030
C	-5.19159	-3.26686	-0.00017
C	-6.69080	-1.36502	0.00021
H	-7.91535	0.38350	0.00065
C	-6.32182	-4.15765	0.00026
C	-7.79153	-2.30267	0.00058
C	-7.63142	-3.67956	0.00063
H	-8.79204	-1.88438	0.00087
H	-8.49388	-4.33415	0.00095
C	-0.23345	6.12923	-0.00021
C	1.04692	5.53466	-0.00030
C	-0.43970	7.55344	0.00023
C	1.29108	4.17865	-0.00068
C	2.16319	6.47659	0.00012
C	0.62918	8.44848	0.00057
H	0.46539	3.47962	-0.00104
C	3.45025	5.97404	0.00020
C	1.90160	7.89866	0.00050
H	0.49347	9.52270	0.00091
H	4.28971	6.66284	0.00053
H	2.76415	8.55591	0.00077
C	2.60541	3.66342	-0.00057
C	3.72175	4.57541	-0.00009

C	2.83932	2.28991	-0.00083
C	5.02063	4.04946	0.00012
C	4.13217	1.77059	-0.00056
H	1.99437	1.60841	-0.00118
C	5.25971	2.66865	-0.00007
H	5.86584	4.73104	0.00048
C	4.35750	0.37695	-0.00066
C	6.56917	2.10726	0.00024
C	5.63111	-0.14866	-0.00025
H	3.49953	-0.28209	-0.00102
C	6.78794	0.74298	0.00018
H	7.42017	2.78176	0.00058
C	5.94114	-1.52578	-0.00015
C	8.12243	0.18629	0.00059
C	7.28942	-2.02889	0.00032
H	8.94741	0.89013	0.00087
C	8.39050	-1.17373	0.00067
H	9.41161	-1.53381	0.00103
C	-5.40170	-5.29828	0.00025
C	-5.21146	-6.67938	0.00055
C	-4.29188	-4.38205	-0.00018
C	-3.89964	-7.12711	0.00047
H	-6.03377	-7.38376	0.00086
C	-2.94416	-4.80199	-0.00029
C	-2.75036	-6.24972	0.00012
H	-3.70244	-8.19346	0.00072
C	-1.85217	-3.96180	-0.00068
C	-1.45954	-6.74239	0.00019
C	-0.53253	-4.46350	-0.00057
H	-1.99388	-2.88924	-0.00102
C	-0.31859	-5.88905	-0.00010
H	-1.30076	-7.81661	0.00051
C	0.56366	-3.60355	-0.00083
C	0.99662	-6.37248	0.00012
H	0.39600	-2.53103	-0.00118
H	1.16442	-7.44523	0.00049
C	1.87010	-4.08781	-0.00056
C	2.10161	-5.51058	-0.00007
C	2.97354	-3.20724	-0.00066
C	3.44855	-5.97490	0.00025
C	4.26990	-3.67394	-0.00025
H	2.78117	-2.14261	-0.00102
C	4.52736	-5.11160	0.00019
H	3.62540	-7.04630	0.00059
C	5.42506	-2.86248	-0.00014
C	5.88973	-5.59619	0.00059
H	6.02760	-6.67183	0.00086
C	7.00217	-4.76925	0.00068
H	8.00028	-5.18889	0.00102
C	6.76152	-3.39595	0.00033

T6 restricted

C	-0.20742	4.56669	-0.00018
C	-1.24378	5.49358	-0.00013
C	-0.93349	6.91373	-0.00008
C	0.40393	7.31298	-0.00008
C	-2.59152	5.08366	-0.00012
C	-2.00771	7.84020	0.00001
C	-3.33085	7.43407	0.00006
C	-3.62305	6.00054	-0.00002
C	-4.99477	5.67762	0.00006
C	-5.99271	6.61414	0.00028
C	-5.73407	8.00177	0.00038
C	-4.41439	8.38204	0.00024
H	-2.81134	4.02360	-0.00013
H	-0.44289	3.50715	-0.00022
H	0.63955	8.37288	-0.00003
H	-1.77767	8.90147	0.00008
H	-6.52597	8.73989	0.00052
H	-4.15626	9.43536	0.00027
C	4.54224	3.45380	-0.00014
C	5.87028	3.83155	-0.00007
H	4.28008	2.40343	-0.00015
C	5.21327	6.19012	0.00000
C	6.96494	2.94465	-0.00003
C	6.22953	5.24935	0.00002
H	5.46735	7.24588	0.00007
C	8.27113	3.35468	0.00016
C	7.61679	5.63258	0.00017
C	8.64068	4.71633	0.00024
H	7.84220	6.69339	0.00027
H	9.67448	5.03765	0.00038
C	-6.03314	4.55943	0.00008
C	-6.25359	3.16759	0.00001
C	-7.04092	5.48532	0.00026
C	-5.26248	2.20659	-0.00032
C	-7.66131	2.76968	0.00022
C	-8.40540	5.12434	0.00042
H	-4.22168	2.50451	-0.00045
C	-7.96773	1.41960	0.00008
C	-8.68692	3.77991	0.00039
H	-9.20041	5.85914	0.00059
H	-9.00893	1.11112	0.00007
H	-9.71822	3.44441	0.00050
C	-5.78593	-5.65861	0.00000
C	-3.38522	-6.13790	-0.00018
C	-4.77268	-6.60171	0.00005
H	-6.82009	-5.98990	0.00027
C	-2.41964	-7.16446	-0.00011
C	-5.05178	-8.01416	0.00029
C	-2.73153	-8.49685	0.00017
H	-6.09304	-8.31732	0.00041
C	-4.06262	-8.96682	0.00037
H	-4.30584	-10.02170	0.00058

C	8.72470	1.88275	0.00019
C	9.79653	0.96522	0.00038
C	7.41419	1.48666	0.00001
C	9.46581	-0.36824	0.00039
H	10.83185	1.28151	0.00055
C	7.00859	0.13753	-0.00005
C	8.10351	-0.83205	0.00019
H	10.24922	-1.11816	0.00056
C	5.69820	-0.29758	-0.00032
C	7.79307	-2.18158	0.00024
C	5.37990	-1.66908	-0.00030
H	4.89033	0.42309	-0.00055
C	6.45412	-2.64798	0.00001
H	8.59743	-2.91110	0.00045
C	0.71978	-5.66062	-0.00038
C	2.75425	-7.61002	0.00026
C	0.38353	-6.99907	-0.00013
H	-0.05898	-4.90845	-0.00066
C	1.43208	-8.01935	0.00019
H	3.54197	-8.35745	0.00051
C	-0.93205	-7.50428	-0.00011
C	1.07007	-9.41283	0.00045
H	1.87628	-10.13821	0.00062
C	-0.23492	-9.84126	0.00047
H	-0.47391	-10.89713	0.00070
C	-1.22976	-8.83999	0.00018
C	3.12033	-6.23951	0.00003
C	4.45029	-5.81662	0.00017
C	2.06422	-5.24062	-0.00032
C	4.79679	-4.45289	-0.00003
H	5.24198	-6.55964	0.00044
C	2.39888	-3.89121	-0.00053
C	6.13026	-4.00685	0.00012
C	3.73149	-3.46356	-0.00039
H	1.60766	-3.14820	-0.00080
H	6.93025	-4.74098	0.00038
C	4.05844	-2.10354	-0.00053
H	3.25918	-1.36919	-0.00075
C	-4.13558	-3.82414	-0.00036
C	-3.85103	-2.46303	-0.00045
C	-5.52044	-4.26523	-0.00013
C	-4.86575	-1.49954	-0.00033
H	-2.81568	-2.13723	-0.00063
C	-6.53512	-3.30618	0.00006
C	-4.56958	-0.13222	-0.00041
C	-6.25483	-1.92764	-0.00005
H	-7.57091	-3.63169	0.00028
C	-5.57118	0.83270	-0.00031
H	-3.53053	0.18162	-0.00059
C	-7.26255	-0.94642	0.00011
C	-6.96401	0.41770	-0.00006
H	-8.30183	-1.26063	0.00032
C	-3.10696	-4.78593	-0.00041

H	-2.07904	-4.44603	-0.00059
C	1.13469	4.96345	-0.00017
C	2.17034	4.02346	-0.00020
C	1.45840	6.38079	-0.00012
C	3.50709	4.40822	-0.00015
H	1.92288	2.96662	-0.00024
C	2.81186	6.76269	-0.00010
C	3.84428	5.82193	-0.00010
H	3.06013	7.81965	-0.00005

T6 unrestricted (S=0)

C	3.19849	3.25074	-0.00003
C	3.16773	4.65513	-0.00002
C	4.41867	5.39098	-0.00001
C	5.62963	4.66671	-0.00000
C	1.95953	5.35273	-0.00002
C	4.37515	6.79381	-0.00000
C	3.16708	7.50252	-0.00000
C	1.92413	6.74774	-0.00001
C	0.75920	7.52352	-0.00001
C	0.76621	8.90427	0.00000
C	1.95032	9.64891	0.00000
C	3.13265	8.92868	0.00000
H	1.03263	4.79339	-0.00003
H	2.26066	2.70436	-0.00004
H	6.56710	5.21415	0.00001
H	5.30946	7.34712	0.00000
H	1.96006	10.73145	0.00001
H	4.08081	9.45517	0.00001
C	5.60914	-0.98564	-0.00002
C	6.79626	-1.71609	-0.00000
H	4.65991	-1.50584	-0.00003
C	8.07174	0.37897	0.00001
C	6.88399	-3.11065	0.00000
C	8.07731	-1.01671	0.00001
H	9.01901	0.90964	0.00002
C	8.09873	-3.80483	0.00002
C	9.29431	-1.76296	0.00003
C	9.32989	-3.15103	0.00003
H	10.22422	-1.20496	0.00004
H	10.27431	-3.68029	0.00005
C	-0.75924	7.52352	-0.00001
C	-1.92417	6.74773	-0.00001
C	-0.76626	8.90427	0.00002
C	-1.95956	5.35272	-0.00003
C	-3.16712	7.50251	0.00002
C	-1.95037	9.64890	0.00006
H	-1.03265	4.79339	-0.00005
C	-4.37519	6.79379	0.00003
C	-3.13270	8.92867	0.00005
H	-1.96011	10.73144	0.00008
H	-5.30950	7.34709	0.00005

H	-4.08086	9.45516	0.00007
C	-8.07174	0.37893	0.00002
C	-6.79625	-1.71612	-0.00001
C	-8.07731	-1.01675	0.00001
H	-9.01901	0.90959	0.00004
C	-6.88397	-3.11068	-0.00001
C	-9.29430	-1.76301	0.00004
C	-8.09871	-3.80487	0.00001
H	-10.22421	-1.20501	0.00006
C	-9.32988	-3.15108	0.00004
H	-10.27429	-3.68034	0.00006
C	7.34296	-5.11221	0.00002
C	7.39096	-6.50543	0.00005
C	6.13545	-4.40670	0.00000
C	6.17046	-7.16747	0.00004
H	8.32102	-7.05953	0.00006
C	4.88359	-5.02774	-0.00000
C	4.91707	-6.48537	0.00002
H	6.15130	-8.25180	0.00005
C	3.65706	-4.36379	-0.00002
C	3.70309	-7.17729	0.00002
C	2.44545	-5.06278	-0.00002
H	3.63389	-3.28158	-0.00004
C	2.45905	-6.51532	-0.00000
H	3.71592	-8.26303	0.00003
C	-3.65704	-4.36380	-0.00003
C	-3.70306	-7.17731	0.00000
C	-4.88357	-5.02777	-0.00001
H	-3.63387	-3.28160	-0.00004
C	-4.91704	-6.48539	0.00000
H	-3.71588	-8.26305	0.00002
C	-6.13542	-4.40673	-0.00001
C	-6.17042	-7.16750	0.00002
H	-6.15125	-8.25183	0.00003
C	-7.39092	-6.50547	0.00002
H	-8.32099	-7.05957	0.00004
C	-7.34293	-5.11225	0.00001
C	-2.45902	-6.51533	-0.00001
C	-1.23419	-7.20177	-0.00000
C	-2.44543	-5.06279	-0.00003
C	0.00002	-6.52913	-0.00001
H	-1.24026	-8.28737	0.00001
C	-1.21881	-4.38920	-0.00004
C	1.23423	-7.20176	0.00000
C	0.00001	-5.07420	-0.00003
H	-1.21327	-3.30382	-0.00005
H	1.24030	-8.28737	0.00002
C	1.21883	-4.38920	-0.00004
H	1.21329	-3.30382	-0.00005
C	-5.60824	0.41538	-0.00002
C	-4.41454	1.13865	-0.00004
C	-6.87570	1.12962	0.00000
C	-4.39697	2.54176	-0.00003

H	-3.47127	0.60178	-0.00006
C	-6.86159	2.52900	0.00001
C	-3.19850	3.25072	-0.00004
C	-5.65908	3.26840	-0.00000
H	-7.80530	3.06556	0.00003
C	-3.16776	4.65512	-0.00002
H	-2.26067	2.70435	-0.00006
C	-5.62966	4.66669	0.00001
C	-4.41870	5.39096	0.00001
H	-6.56713	5.21412	0.00004
C	-5.60914	-0.98566	-0.00003
H	-4.65990	-1.50586	-0.00005
C	4.39696	2.54178	-0.00002
C	4.41453	1.13867	-0.00003
C	5.65906	3.26843	-0.00001
C	5.60824	0.41540	-0.00002
H	3.47126	0.60180	-0.00004
C	6.86158	2.52904	0.00000
C	6.87569	1.12965	-0.00000
H	7.80529	3.06560	0.00001

T6 unrestricted (S=1)

C	-3.24148	3.18299	0.00002
C	-4.63015	3.15389	0.00001
C	-5.37180	4.40397	-0.00001
C	-4.67783	5.59942	-0.00001
C	-5.33329	1.93527	0.00001
C	-6.80632	4.33601	-0.00002
C	-7.48525	3.14484	-0.00002
C	-6.72006	1.89272	-0.00000
C	-7.49149	0.73174	-0.00001
C	-8.92734	0.72640	0.00000
C	-9.66361	1.92935	-0.00003
C	-8.93846	3.09508	-0.00004
H	-4.76719	1.01311	0.00002
H	-2.69083	2.24767	0.00003
H	-5.22855	6.53524	-0.00003
H	-7.36260	5.26875	-0.00004
H	-10.74617	1.95007	-0.00005
H	-9.45838	4.04708	-0.00007
C	0.98900	5.60921	0.00002
C	1.71148	6.79580	0.00001
H	1.51154	4.66127	0.00003
C	-0.38619	8.06329	-0.00002
C	3.11116	6.88708	0.00001
C	1.00940	8.07285	-0.00001
H	-0.91971	9.00908	-0.00003
C	3.79700	8.09427	0.00001
C	1.75517	9.29353	-0.00003
C	3.13843	9.32939	-0.00002
H	1.19565	10.22259	-0.00005
H	3.66811	10.27356	-0.00004

C	-7.49219	-0.72454	0.00000
C	-6.72188	-1.88627	-0.00000
C	-8.92803	-0.71782	0.00001
C	-5.33516	-1.93016	-0.00003
C	-7.48828	-3.13765	0.00003
C	-9.66546	-1.92006	0.00006
H	-4.76817	-1.00854	-0.00006
C	-6.81049	-4.32948	0.00003
C	-8.94144	-3.08649	0.00007
H	-10.74804	-1.93974	0.00010
H	-7.36768	-5.26168	0.00006
H	-9.46228	-4.03799	0.00011
C	-0.39392	-8.06292	0.00002
C	1.70495	-6.79742	-0.00001
C	1.00165	-8.07380	0.00002
H	-0.92834	-9.00820	0.00004
C	3.10455	-6.89004	-0.00001
C	1.74625	-9.29520	0.00004
C	3.78923	-8.09790	0.00000
H	1.18584	-10.22372	0.00006
C	3.12948	-9.33239	0.00003
H	3.65826	-10.27707	0.00006
C	5.11451	7.33958	0.00001
C	6.50570	7.38911	0.00005
C	4.41122	6.13346	0.00001
C	7.16992	6.16739	0.00005
H	7.05942	8.31941	0.00007
C	5.03155	4.88324	0.00001
C	6.48886	4.91636	0.00003
H	8.25426	6.14970	0.00008
C	4.36705	3.65452	-0.00001
C	7.18059	3.69931	0.00003
C	5.06529	2.44447	-0.00000
H	3.28483	3.63162	-0.00002
C	6.51850	2.45753	0.00001
H	8.26634	3.71195	0.00004
C	4.36354	-3.65871	-0.00002
C	7.17704	-3.70620	-0.00002
C	5.02687	-4.88806	-0.00002
H	3.28134	-3.63477	-0.00002
C	6.48414	-4.92258	-0.00002
H	8.26278	-3.71988	-0.00002
C	4.40533	-6.13769	-0.00001
C	7.16399	-6.17427	-0.00002
H	8.24835	-6.15762	-0.00003
C	6.49860	-7.39535	-0.00001
H	7.05143	-8.32619	-0.00002
C	5.10746	-7.34448	0.00000
C	6.51615	-2.46379	-0.00001
C	7.20314	-1.23747	-0.00001
C	5.06294	-2.44934	-0.00002
C	6.53143	-0.00313	-0.00000
H	8.28874	-1.24413	0.00000

C	4.39014	-1.22071	-0.00002
C	7.20432	1.23056	0.00001
C	5.07545	-0.00244	-0.00001
H	3.30476	-1.21463	-0.00003
H	8.28992	1.23618	0.00002
C	4.39131	1.21649	-0.00002
H	3.30592	1.21145	-0.00003
C	-0.41752	-5.60605	-0.00003
C	-1.13776	-4.40704	-0.00005
C	-1.13487	-6.86550	0.00000
C	-2.53141	-4.38971	-0.00003
H	-0.59706	-3.46590	-0.00007
C	-2.54400	-6.84010	0.00001
C	-3.24456	-3.17989	-0.00005
C	-3.26163	-5.64378	-0.00000
H	-3.08485	-7.78158	0.00003
C	-4.63320	-3.14946	-0.00002
H	-2.69300	-2.24510	-0.00007
C	-4.68322	-5.59494	0.00002
C	-5.37604	-4.39882	0.00001
H	-5.23484	-6.53024	0.00004
C	0.98360	-5.61014	-0.00003
H	1.50704	-4.66270	-0.00006
C	-2.52717	4.39213	0.00001
C	-1.13350	4.40813	0.00002
C	-3.25620	5.64689	-0.00000
C	-0.41212	5.60645	0.00001
H	-0.59371	3.46647	0.00003
C	-2.53743	6.84253	-0.00001
C	-1.12827	6.86658	-0.00000
H	-3.07738	7.78453	-0.00002

T6 unrestricted (S=2)

C	-3.25022	3.19602	-0.00000
C	-4.67092	3.15563	-0.00001
C	-5.40801	4.40763	-0.00002
C	-4.67033	5.62634	-0.00002
C	-5.35460	1.95850	-0.00000
C	-6.79501	4.36950	-0.00003
C	-7.51796	3.15056	-0.00002
C	-6.76595	1.91359	-0.00001
C	-7.53089	0.75392	-0.00000
C	-8.92689	0.75977	-0.00001
C	-9.66296	1.93479	-0.00003
C	-8.93092	3.12316	-0.00003
H	-4.79487	1.03165	0.00001
H	-2.70538	2.25721	0.00001
H	-5.21882	6.56313	-0.00003
H	-7.34956	5.30315	-0.00003
H	-10.74542	1.95130	-0.00003
H	-9.45640	4.07200	-0.00004
C	0.97829	5.60189	0.00001

C	1.72797	6.80120	0.00001
H	1.49849	4.65234	0.00001
C	-0.39208	8.05754	-0.00001
C	3.10919	6.88232	0.00001
C	1.03295	8.07631	-0.00000
H	-0.92094	9.00595	-0.00001
C	3.80799	8.10274	0.00001
C	1.75685	9.27632	-0.00000
C	3.16464	9.31851	0.00000
H	1.20057	10.20745	-0.00001
H	3.68793	10.26614	0.00000
C	-7.53089	-0.75391	0.00000
C	-6.76595	-1.91359	0.00001
C	-8.92689	-0.75977	0.00001
C	-5.35460	-1.95850	-0.00000
C	-7.51796	-3.15055	0.00002
C	-9.66296	-1.93478	0.00003
H	-4.79487	-1.03165	-0.00001
C	-6.79502	-4.36949	0.00003
C	-8.93092	-3.12315	0.00004
H	-10.74542	-1.95130	0.00004
H	-7.34956	-5.30314	0.00004
H	-9.45640	-4.07199	0.00005
C	-0.39209	-8.05754	0.00001
C	1.72796	-6.80120	-0.00001
C	1.03295	-8.07631	0.00000
H	-0.92094	-9.00595	0.00002
C	3.10919	-6.88232	-0.00001
C	1.75684	-9.27632	0.00001
C	3.80799	-8.10274	-0.00001
H	1.20056	-10.20745	0.00001
C	3.16463	-9.31851	0.00000
H	3.68793	-10.26614	0.00000
C	5.11778	7.33103	0.00002
C	6.51867	7.38114	0.00003
C	4.41535	6.13835	0.00001
C	7.17899	6.16804	0.00003
H	7.06879	8.31344	0.00003
C	5.03773	4.87814	0.00001
C	6.49403	4.91116	0.00002
H	8.26333	6.14733	0.00003
C	4.37172	3.65936	0.00001
C	7.18573	3.70064	0.00002
C	5.07000	2.44335	0.00001
H	3.28940	3.63863	0.00000
C	6.52205	2.45646	0.00001
H	8.27145	3.71259	0.00002
C	4.37172	-3.65937	-0.00001
C	7.18573	-3.70064	-0.00001
C	5.03773	-4.87814	-0.00001
H	3.28940	-3.63863	-0.00001
C	6.49403	-4.91116	-0.00002
H	8.27145	-3.71260	-0.00001

C	4.41534	-6.13835	-0.00001
C	7.17899	-6.16804	-0.00002
H	8.26333	-6.14734	-0.00002
C	6.51867	-7.38114	-0.00002
H	7.06878	-8.31345	-0.00002
C	5.11778	-7.33103	-0.00001
C	6.52205	-2.45647	-0.00001
C	7.20926	-1.23321	-0.00000
C	5.07000	-2.44336	-0.00001
C	6.53564	-0.00000	0.00000
H	8.29479	-1.23914	-0.00000
C	4.39544	-1.21936	-0.00001
C	7.20926	1.23321	0.00001
C	5.08046	-0.00000	-0.00000
H	3.31008	-1.21428	-0.00001
H	8.29480	1.23914	0.00001
C	4.39544	1.21936	0.00000
H	3.31008	1.21428	-0.00000
C	-0.40398	-5.60744	-0.00000
C	-1.14297	-4.40715	-0.00001
C	-1.11976	-6.88033	0.00001
C	-2.54408	-4.38632	-0.00000
H	-0.60596	-3.46398	-0.00002
C	-2.54093	-6.85340	0.00001
C	-3.25022	-3.19602	-0.00000
C	-3.27603	-5.65888	0.00001
H	-3.07637	-7.79761	0.00002
C	-4.67092	-3.15562	0.00000
H	-2.70538	-2.25721	-0.00001
C	-4.67033	-5.62634	0.00002
C	-5.40802	-4.40763	0.00002
H	-5.21882	-6.56313	0.00003
C	0.97829	-5.60189	-0.00001
H	1.49849	-4.65234	-0.00002
C	-2.54408	4.38632	-0.00000
C	-1.14297	4.40715	0.00000
C	-3.27603	5.65888	-0.00001
C	-0.40397	5.60744	0.00000
H	-0.60596	3.46398	0.00001
C	-2.54092	6.85340	-0.00001
C	-1.11976	6.88033	-0.00001
H	-3.07636	7.79761	-0.00002

T6 unrestricted (S=3)

C	-3.25366	3.18664	-0.00002
C	-4.67131	3.14403	-0.00001
C	-5.41251	4.39567	-0.00000
C	-4.67805	5.61552	0.00000
C	-5.35336	1.94536	-0.00001
C	-6.79845	4.35404	0.00000
C	-7.52077	3.13193	0.00000
C	-6.76631	1.89689	-0.00001

C	-7.52768	0.73674	-0.00000
C	-8.92706	0.73964	0.00000
C	-9.66392	1.91164	0.00001
C	-8.93151	3.10249	0.00001
H	-4.79188	1.01966	-0.00002
H	-2.70651	2.24934	-0.00003
H	-5.22938	6.55057	0.00001
H	-7.35553	5.28613	0.00001
H	-10.74635	1.92745	0.00002
H	-9.45874	4.05035	0.00001
C	0.96790	5.61144	-0.00001
C	1.71234	6.81435	-0.00000
H	1.49296	4.66463	-0.00002
C	-0.40540	8.06215	0.00001
C	3.09661	6.89911	0.00000
C	1.01472	8.08268	0.00001
H	-0.93743	9.00877	0.00002
C	3.78945	8.11676	0.00001
C	1.73969	9.29203	0.00002
C	3.13823	9.33717	0.00002
H	1.17900	10.22049	0.00003
H	3.66082	10.28520	0.00003
C	-7.52451	-0.76841	-0.00000
C	-6.75827	-1.92535	-0.00001
C	-8.92387	-0.77719	0.00001
C	-5.34513	-1.96787	-0.00002
C	-7.50753	-3.16355	0.00001
C	-9.65579	-1.95229	0.00003
H	-4.78755	-1.03982	-0.00003
C	-6.78006	-4.38261	0.00001
C	-8.91838	-3.14004	0.00002
H	-10.73815	-1.97266	0.00003
H	-7.33323	-5.31703	0.00002
H	-9.44162	-4.09012	0.00003
C	-0.37147	-8.06378	0.00001
C	1.74100	-6.80707	-0.00001
C	1.04873	-8.07833	0.00001
H	-0.89950	-9.01263	0.00002
C	3.12562	-6.88601	-0.00000
C	1.77878	-9.28462	0.00002
C	3.82358	-8.10074	0.00001
H	1.22200	-10.21543	0.00003
C	3.17750	-9.32388	0.00002
H	3.70407	-10.26970	0.00003
C	5.10369	7.36120	0.00001
C	6.48691	7.41354	0.00002
C	4.40138	6.15026	-0.00000
C	7.15216	6.18367	0.00002
H	7.04191	8.34296	0.00003
C	5.02590	4.91110	-0.00000
C	6.47247	4.94733	0.00001
H	8.23667	6.16669	0.00003
C	4.36149	3.66285	-0.00001

C	7.17005	3.71059	0.00001
C	5.05856	2.47289	-0.00001
H	3.27909	3.63973	-0.00002
C	6.51346	2.48927	-0.00000
H	8.25580	3.72739	0.00002
C	4.37688	-3.64447	-0.00002
C	7.18561	-3.68039	0.00000
C	5.04653	-4.88991	-0.00001
H	3.29439	-3.62590	-0.00002
C	6.49324	-4.92006	0.00000
H	8.27143	-3.69261	0.00001
C	4.42723	-6.13169	-0.00001
C	7.17813	-6.15352	0.00001
H	8.26256	-6.13198	0.00002
C	6.51805	-7.38618	0.00002
H	7.07696	-8.31326	0.00003
C	5.13462	-7.33967	0.00001
C	6.52389	-2.46184	-0.00000
C	7.20782	-1.21354	-0.00000
C	5.06892	-2.45159	-0.00002
C	6.53735	0.01375	-0.00001
H	8.29331	-1.21879	0.00001
C	4.39210	-1.20564	-0.00002
C	7.20265	1.24386	0.00000
C	5.06918	0.01066	-0.00002
H	3.30679	-1.20463	-0.00003
H	8.28810	1.25369	0.00001
C	4.38699	1.22410	-0.00002
H	3.30168	1.21852	-0.00003
C	-0.38754	-5.61581	-0.00001
C	-1.13315	-4.41038	-0.00002
C	-1.10119	-6.88471	0.00000
C	-2.52597	-4.39426	-0.00002
H	-0.59584	-3.46740	-0.00003
C	-2.52348	-6.85910	0.00001
C	-3.24023	-3.20031	-0.00002
C	-3.25722	-5.66741	-0.00000
H	-3.05789	-7.80394	0.00002
C	-4.65805	-3.16365	-0.00001
H	-2.69703	-2.26071	-0.00003
C	-4.65438	-5.63515	0.00001
C	-5.39396	-4.41841	0.00000
H	-5.20177	-6.57252	0.00002
C	0.99150	-5.60731	-0.00002
H	1.51257	-4.65830	-0.00003
C	-2.54444	4.38359	-0.00001
C	-1.15169	4.40558	-0.00002
C	-3.28104	5.65366	-0.00000
C	-0.41116	5.61414	-0.00001
H	-0.61041	3.46487	-0.00003
C	-2.55233	6.84842	0.00000
C	-1.13016	6.88002	0.00000
H	-3.09071	7.79100	0.00001

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C	-0.61937	5.64150	-0.00015
C	0.06474	6.84977	-0.00009
C	-0.68483	8.09695	-0.00001
C	-2.07692	8.04960	0.00000
C	1.47439	6.89493	-0.00010
C	0.03686	9.31995	0.00005
C	1.41876	9.35900	0.00005
C	2.15613	8.09394	-0.00002
C	3.55933	8.22993	-0.00001
C	4.20188	9.43768	0.00008
C	3.51138	10.66980	0.00015
C	2.14029	10.60602	0.00014
H	2.02357	5.96180	-0.00016
H	-0.05736	4.71290	-0.00021
H	-2.63882	8.97859	0.00006
H	-0.52160	10.25124	0.00011
H	4.02490	11.62283	0.00022
H	1.55694	11.52021	0.00019
C	-6.82723	1.76272	-0.00010
C	-8.20467	1.68875	-0.00003
H	-6.23793	0.85438	-0.00015
C	-8.35392	4.13251	0.00005
C	-8.95379	0.49436	-0.00001
C	-9.00667	2.91384	0.00005
H	-8.93734	5.04837	0.00010
C	-10.32139	0.45935	0.00007
C	-10.44476	2.82580	0.00013
C	-11.11472	1.62776	0.00015
H	-11.00179	3.75628	0.00018
H	-12.19677	1.59448	0.00021
C	4.90453	7.50631	0.00000
C	5.56461	6.26042	-0.00001
C	5.55770	8.70840	0.00009
C	4.94054	5.03027	-0.00008
C	7.02649	6.34307	0.00008
C	6.96614	8.81175	0.00018
H	3.85929	4.97350	-0.00015
C	7.75608	5.16872	0.00009
C	7.66897	7.63272	0.00017
H	7.47820	9.76556	0.00025
H	8.84092	5.21664	0.00015
H	8.75329	7.65014	0.00023
C	8.05414	-4.69283	0.00005
C	5.93223	-5.91461	-0.00003
C	7.39650	-5.90892	0.00004
H	9.13989	-4.67527	0.00011
C	5.34807	-7.19763	-0.00002
C	8.11526	-7.15760	0.00012
C	6.07236	-8.35822	0.00006
H	9.19866	-7.10976	0.00017
C	7.48457	-8.37671	0.00013
H	8.05298	-9.29806	0.00019

C	-10.27535	-1.07954	0.00007
C	-10.99726	-2.29343	0.00015
C	-8.90809	-1.03242	-0.00000
C	-10.25657	-3.44908	0.00015
H	-12.07936	-2.32525	0.00021
C	-8.08880	-2.17963	-0.00001
C	-8.81577	-3.45069	0.00007
H	-10.75672	-4.41132	0.00020
C	-6.70961	-2.17070	-0.00007
C	-8.09097	-4.62808	0.00008
C	-5.96571	-3.36901	-0.00006
H	-6.17589	-1.22863	-0.00014
C	-6.67093	-4.64176	0.00003
H	-8.61845	-5.57726	0.00014
C	1.88644	-6.79267	-0.00009
C	0.59791	-9.29999	0.00006
C	2.63951	-7.94849	-0.00002
H	2.37812	-5.82800	-0.00014
C	1.97966	-9.25565	0.00005
H	0.09666	-10.26329	0.00012
C	4.04850	-8.00031	-0.00002
C	2.77478	-10.45713	0.00011
H	2.24721	-11.40463	0.00016
C	4.14727	-10.43853	0.00012
H	4.71698	-11.35907	0.00018
C	4.76254	-9.16731	0.00006
C	-0.19623	-8.12274	0.00001
C	-1.58864	-8.15970	0.00003
C	0.47649	-6.83260	-0.00007
H	-2.09327	-9.12101	0.00009
C	-5.93370	-5.82375	0.00005
H	-6.45730	-6.77485	0.00011
C	-4.57735	-3.35728	-0.00012
H	-4.05413	-2.40628	-0.00018
C	5.90146	-3.48132	-0.00009
C	5.19734	-2.28467	-0.00014
C	7.35625	-3.45599	-0.00001
H	4.11214	-2.30687	-0.00021
C	8.01158	-2.22675	0.00002
C	5.04981	2.59223	-0.00013
H	9.09705	-2.20482	0.00008
C	5.68032	3.82934	-0.00007
H	3.96527	2.54866	-0.00020
C	7.86229	2.70466	0.00004
C	7.13395	3.89209	0.00002
H	8.94711	2.74847	0.00010
C	5.23521	-4.72446	-0.00010
H	4.15250	-4.73296	-0.00016
C	-4.76986	3.07553	-0.00015
C	-6.15658	3.00354	-0.00009
H	-4.19027	2.15780	-0.00021
C	-6.27267	5.45552	0.00000
C	-6.93725	4.23140	-0.00002

H	-6.85261	6.37336	0.00006
C	7.23178	1.44349	-0.00002
C	7.94911	0.23937	0.00002
C	5.77723	1.39302	-0.00011
C	7.30598	-1.00594	-0.00003
H	9.03426	0.27231	0.00008
C	5.13500	0.15405	-0.00015
C	5.85103	-1.04380	-0.00011
H	4.05013	0.12109	-0.00022
C	-2.78109	6.82814	-0.00005
C	-4.18101	6.76261	-0.00001
C	-2.02086	5.58693	-0.00013
C	-4.86526	5.53956	-0.00005
H	-4.75197	7.68603	0.00005
C	-2.70039	4.36797	-0.00017
C	-4.09457	4.30485	-0.00013
H	-2.12958	3.44482	-0.00023
C	-1.68184	-5.69811	-0.00009
C	-2.43387	-4.52241	-0.00013
C	-2.36544	-6.98304	-0.00001
C	-3.82923	-4.54369	-0.00009
H	-1.91997	-3.56641	-0.00020
C	-3.76676	-7.00233	0.00003
H	-4.28082	-7.95858	0.00009
C	-0.27959	-5.66785	-0.00012
H	0.22508	-4.70688	-0.00018
C	-4.52377	-5.82278	-0.00000

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C	-3.54754	4.41930	-0.00002
C	-3.61290	5.82584	-0.00001
C	-4.91202	6.47213	0.00000
C	-6.07091	5.66319	0.00001
C	-2.45823	6.60497	-0.00002
C	-4.96899	7.87167	0.00001
C	-3.81285	8.66623	0.00001
C	-2.52047	8.00193	-0.00001
C	-1.41477	8.85789	-0.00000
C	-1.52220	10.23654	0.00001
C	-2.75460	10.89389	0.00002
C	-3.88265	10.08902	0.00002
H	-1.49371	6.11293	-0.00003
H	-2.57394	3.93950	-0.00003
H	-7.04407	6.14431	0.00002
H	-5.94009	8.35750	0.00002
H	-2.84230	11.97291	0.00003
H	-4.86652	10.54534	0.00003
C	-6.69390	-2.18511	-0.00001
C	-7.82443	-3.00784	0.00000
H	-5.70785	-2.63216	-0.00002
C	-9.25160	-1.01243	0.00002
C	-7.80602	-4.40329	0.00000

C	-9.15278	-2.40870	0.00002
H	-10.23647	-0.55528	0.00003
C	-8.96609	-5.18630	0.00002
C	-10.30925	-3.24017	0.00003
C	-10.24135	-4.62860	0.00003
H	-11.27813	-2.75291	0.00004
H	-11.14339	-5.22721	0.00004
C	0.09937	8.96940	-0.00000
C	1.31864	8.28470	-0.00001
C	0.00355	10.34891	0.00001
C	1.46196	6.89366	-0.00002
C	2.49961	9.13141	0.00001
C	1.12625	11.17983	0.00002
H	0.58006	6.26546	-0.00003
C	3.75975	8.51502	0.00001
C	2.36012	10.54902	0.00002
H	1.05480	12.26004	0.00003
H	4.64910	9.13800	0.00002
H	3.26648	11.14460	0.00003
C	9.30018	0.35623	0.00002
C	8.18150	-1.82718	0.00000
C	9.40746	-1.03944	0.00002
H	10.20726	0.95302	0.00003
C	8.36804	-3.21019	0.00000
C	10.67344	-1.69215	0.00003
C	9.63046	-3.81441	0.00002
H	11.56031	-1.06797	0.00004
C	10.81010	-3.07552	0.00003
H	11.79021	-3.53528	0.00005
C	-8.11577	-6.43424	0.00002
C	-8.06470	-7.82666	0.00003
C	-6.96324	-5.64287	0.00000
C	-6.79940	-8.39888	0.00002
H	-8.95285	-8.44567	0.00004
C	-5.67068	-6.17240	-0.00000
C	-5.60051	-7.62765	0.00001
H	-6.70140	-9.47896	0.00003
C	-4.49203	-5.42257	-0.00002
C	-4.33869	-8.23174	0.00001
C	-3.23624	-6.03393	-0.00002
H	-4.54623	-4.34127	-0.00003
C	-3.14777	-7.48345	-0.00000
H	-4.27444	-9.31565	0.00002
C	5.23932	-4.70463	-0.00002
C	5.49984	-7.50582	0.00001
C	6.51526	-5.27340	-0.00000
H	5.13429	-3.62710	-0.00003
C	6.65941	-6.72317	0.00001
H	5.59533	-8.58743	0.00002
C	7.71621	-4.55997	0.00000
C	7.95852	-7.31018	0.00002
H	8.02011	-8.39294	0.00003
C	9.12617	-6.55845	0.00003

H	10.09552	-7.04049	0.00004
C	8.97241	-5.17361	0.00002
C	4.21201	-6.94036	-0.00000
C	3.04176	-7.72000	-0.00000
C	4.08675	-5.49359	-0.00002
H	3.13218	-8.80183	0.00001
C	-1.87577	-8.08291	-0.00000
H	-1.80637	-9.16630	0.00001
C	-2.05592	-5.27611	-0.00003
H	-2.12620	-4.19297	-0.00003
C	6.84469	0.21351	-0.00001
C	5.59900	0.85742	-0.00002
C	8.05739	1.01465	0.00000
H	4.69572	0.25562	-0.00003
C	7.94213	2.41503	0.00001
C	2.86022	4.89133	-0.00003
H	8.84620	3.01595	0.00002
C	2.71844	6.29228	-0.00002
H	1.96759	4.27384	-0.00004
C	5.17366	6.49222	0.00000
C	3.90862	7.12227	-0.00000
H	6.06566	7.11096	0.00002
C	6.94246	-1.17941	-0.00001
H	6.03274	-1.76637	-0.00003
C	-5.66414	0.02706	-0.00002
C	-6.80174	-0.79290	-0.00001
H	-4.68226	-0.43551	-0.00003
C	-8.21069	1.22346	0.00001
C	-8.11897	-0.17866	0.00001
H	-9.19323	1.68508	0.00002
C	5.31111	5.10226	-0.00000
C	6.56822	4.46029	0.00000
C	4.10872	4.27862	-0.00002
C	6.69512	3.06454	-0.00000
H	7.46630	5.07004	0.00002
C	4.23790	2.87958	-0.00003
C	5.48530	2.25080	-0.00002
H	3.34002	2.26993	-0.00004
C	-6.00287	4.26807	-0.00000
C	-7.15210	3.44840	0.00001
C	-4.69257	3.62999	-0.00002
C	-7.07261	2.04913	-0.00000
H	-8.12999	3.91965	0.00002
C	-4.61486	2.22719	-0.00003
C	-5.75638	1.42202	-0.00002
H	-3.63717	1.75603	-0.00004
C	1.64784	-5.69377	-0.00002
C	0.37673	-5.10672	-0.00003
C	1.76126	-7.14550	-0.00001
C	-0.79442	-5.87400	-0.00002
H	0.29681	-4.02433	-0.00004
C	0.58389	-7.91345	-0.00001
H	0.66382	-8.99606	0.00000

C	2.80796	-4.91721	-0.00003
H	2.71843	-3.83549	-0.00003
C	-0.69347	-7.32667	-0.00001

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C	2.42857	5.11719	-0.00001
C	3.68219	5.78718	-0.00001
C	3.69992	7.24010	-0.00000
C	2.45303	7.93143	0.00000
C	4.87047	5.08784	-0.00001
C	4.92127	7.89768	0.00000
C	6.15387	7.20137	0.00000
C	6.11667	5.75065	-0.00000
C	7.35618	5.12785	0.00000
C	8.56192	5.82571	0.00001
C	8.61855	7.20978	0.00001
C	7.39237	7.87946	0.00001
H	4.84572	4.00518	-0.00001
H	2.42096	4.03169	-0.00001
H	2.46412	9.01709	0.00000
H	4.93709	8.98356	0.00001
H	9.55013	7.76132	0.00001
H	7.37804	8.96393	0.00001
C	-4.87698	5.08158	-0.00001
C	-6.12408	5.74279	-0.00000
H	-4.85085	3.99896	-0.00001
C	-4.93140	7.89136	0.00000
C	-7.36276	5.11841	0.00000
C	-6.16313	7.19347	0.00000
H	-4.94863	8.97722	0.00001
C	-8.56943	5.81474	0.00001
C	-7.40248	7.86996	0.00001
C	-8.62783	7.19870	0.00001
H	-7.38955	8.95445	0.00001
H	-9.56011	7.74906	0.00001
C	8.12149	3.81784	0.00000
C	8.02694	2.40769	0.00000
C	9.31274	4.49469	0.00001
C	6.85034	1.69220	-0.00001
C	9.31324	1.70867	0.00001
C	10.56604	3.83776	0.00001
H	5.90114	2.21298	-0.00001
C	9.31735	0.32795	0.00001
C	10.54048	2.46777	0.00001
H	11.50374	4.37863	0.00002
H	10.26517	-0.20193	0.00001
H	11.47045	1.90972	0.00001
C	4.38750	-8.21684	0.00000
C	1.94023	-8.14247	-0.00000
C	3.18901	-8.90660	0.00000
H	5.32068	-8.77212	0.00001
C	0.76937	-8.92748	-0.00000

C	3.14521	-10.34646	0.00001
C	0.77630	-10.29576	0.00001
H	4.09235	-10.87464	0.00001
C	1.96819	-11.05295	0.00001
H	1.96821	-12.13553	0.00002
C	-9.31852	4.48276	0.00001
C	-10.57097	3.82421	0.00001
C	-8.12640	3.80745	0.00000
C	-10.54365	2.45426	0.00001
H	-11.50936	4.36388	0.00002
C	-8.03003	2.39742	0.00000
C	-9.31543	1.69673	0.00001
H	-11.47290	1.89502	0.00001
C	-6.85251	1.68345	-0.00001
C	-9.31776	0.31602	0.00001
C	-6.84704	0.27071	-0.00001
H	-5.90399	2.20546	-0.00001
C	-8.11518	-0.44219	0.00000
H	-10.26490	-0.21509	0.00001
C	-1.96366	-6.76559	-0.00001
C	-4.37695	-8.22240	0.00000
C	-1.92977	-8.14492	-0.00000
H	-1.03863	-6.20290	-0.00001
C	-3.17759	-8.91063	0.00000
H	-5.30942	-8.77887	0.00001
C	-0.75792	-8.92844	-0.00000
C	-3.13196	-10.35043	0.00001
H	-4.07844	-10.87982	0.00001
C	-1.95405	-11.05543	0.00001
H	-1.95270	-12.13801	0.00002
C	-0.76311	-10.29674	0.00001
C	-4.43411	-6.80388	0.00000
C	-5.63873	-6.10342	0.00000
C	-3.18420	-6.05957	-0.00001
H	-6.57313	-6.65626	0.00001
C	-8.10933	-1.83371	0.00000
H	-9.05435	-2.36818	0.00001
C	-5.65999	-0.44657	-0.00001
H	-4.71541	0.08815	-0.00001
C	3.19200	-6.05554	-0.00001
C	3.22195	-4.66668	-0.00001
C	4.44286	-6.79824	0.00000
H	2.28699	-4.11532	-0.00002
C	5.64658	-6.09624	0.00000
C	5.66056	-0.43937	-0.00001
H	6.58170	-6.64788	0.00001
C	6.84669	0.27945	-0.00001
H	4.71530	0.09413	-0.00001
C	8.11169	-1.82334	0.00000
C	8.11575	-0.43180	0.00000
H	9.05741	-2.35659	0.00001
C	1.97235	-6.76311	-0.00001
H	1.04661	-6.20160	-0.00001

C	-2.43513	5.11406	-0.00001
C	-3.68961	5.78244	-0.00001
H	-2.42612	4.02857	-0.00001
C	-2.46323	7.92828	0.00000
C	-3.70922	7.23535	-0.00000
H	-2.47572	9.01392	0.00000
C	6.91141	-2.56531	-0.00000
C	6.88934	-3.96565	0.00000
C	5.64791	-1.84343	-0.00001
C	5.68713	-4.68754	-0.00000
H	7.82979	-4.50806	0.00001
C	4.45079	-2.55862	-0.00001
C	4.42976	-3.95507	-0.00001
H	3.51065	-2.01625	-0.00002
C	1.23377	7.26825	-0.00000
C	-0.00512	7.94357	-0.00000
C	1.22849	5.80063	-0.00001
C	-1.24307	7.26667	-0.00000
H	-0.00581	9.02909	0.00000
C	-0.00329	5.12373	-0.00001
C	-1.23589	5.79904	-0.00001
H	-0.00259	4.03846	-0.00001
C	-4.42465	-3.96068	-0.00001
C	-4.44749	-2.56426	-0.00001
C	-5.68108	-4.69478	-0.00000
C	-5.64552	-1.85062	-0.00001
H	-3.50804	-2.02067	-0.00002
C	-6.88422	-3.97444	0.00000
H	-7.82397	-4.51806	0.00001
C	-3.21593	-4.67074	-0.00001
H	-2.28168	-4.11819	-0.00002
C	-6.90809	-2.57413	-0.00000

T7 unrestricted (S=2)

C	-0.45959	5.64193	-0.00007
C	0.28724	6.84750	-0.00004
C	-0.42342	8.11314	0.00001
C	-1.85268	8.08689	0.00001
C	1.67007	6.83931	-0.00004
C	0.30175	9.29250	0.00005
C	1.71882	9.30764	0.00005
C	2.41306	8.03555	0.00000
C	3.80285	8.11988	0.00002
C	4.49200	9.33157	0.00007
C	3.84313	10.55670	0.00011
C	2.44785	10.51704	0.00010
H	2.19103	5.89000	-0.00007
H	0.07682	4.69825	-0.00010
H	-2.38583	9.03264	0.00005
H	-0.22827	10.24035	0.00008
H	4.37044	11.50214	0.00015
H	1.88875	11.44645	0.00013

C	-6.77260	1.95431	-0.00006
C	-8.18082	1.90424	-0.00003
H	-6.20852	1.02990	-0.00009
C	-8.22496	4.35823	0.00001
C	-8.94401	0.74007	-0.00002
C	-8.93903	3.13847	0.00001
H	-8.78344	5.28955	0.00004
C	-10.33577	0.74265	0.00003
C	-10.35481	3.10546	0.00006
C	-11.07916	1.91645	0.00007
H	-10.88334	4.05257	0.00008
H	-12.16168	1.92635	0.00011
C	5.11236	7.37046	0.00001
C	5.73851	6.12020	-0.00000
C	5.81096	8.57091	0.00007
C	5.07775	4.88836	-0.00005
C	7.19238	6.15971	0.00004
C	7.20410	8.62780	0.00011
H	3.99533	4.86266	-0.00008
C	7.89003	4.94356	0.00004
C	7.87147	7.41113	0.00009
H	7.75213	9.56138	0.00015
H	8.97570	4.96067	0.00007
H	8.95588	7.39555	0.00012
C	7.90744	-4.91565	0.00002
C	5.76011	-6.09990	-0.00003
C	7.21410	-6.13428	0.00002
H	8.99317	-4.92892	0.00005
C	5.13838	-7.35238	-0.00001
C	7.89762	-7.38329	0.00007
C	5.84123	-8.55035	0.00005
H	8.98197	-7.36387	0.00011
C	7.23455	-8.60232	0.00009
H	7.78589	-9.53395	0.00014
C	-10.33306	-0.77919	0.00006
C	-11.07227	-1.95563	0.00011
C	-8.94132	-0.77167	0.00001
C	-10.34371	-3.14205	0.00010
H	-12.15476	-1.96937	0.00015
C	-8.17399	-1.93313	-0.00001
C	-8.92782	-3.17003	0.00005
H	-10.86886	-4.09104	0.00014
C	-6.76559	-1.97819	-0.00006
C	-8.20943	-4.38724	0.00006
C	-6.08293	-3.17793	-0.00005
H	-6.20481	-1.05178	-0.00011
C	-6.82141	-4.42625	0.00001
H	-8.76459	-5.32054	0.00010
C	1.69429	-6.83340	-0.00006
C	0.33459	-9.29138	0.00007
C	2.44148	-8.02702	-0.00001
H	2.21190	-5.88226	-0.00012
C	1.75171	-9.30154	0.00006

H	-0.19208	-10.24110	0.00012
C	3.83154	-8.10643	0.00000
C	2.48500	-10.50835	0.00012
H	1.92918	-11.43973	0.00017
C	3.88041	-10.54310	0.00012
H	4.41107	-11.48666	0.00018
C	4.52496	-9.31568	0.00006
C	-0.39472	-8.11458	0.00002
C	-1.82407	-8.09336	0.00004
C	0.31150	-6.84645	-0.00005
H	-2.35387	-9.04098	0.00009
C	-6.08677	-5.64776	0.00003
H	-6.63786	-6.58312	0.00008
C	-4.66096	-3.22243	-0.00010
H	-4.11338	-2.28512	-0.00015
C	5.79400	-3.66345	-0.00007
C	5.12204	-2.42904	-0.00010
C	7.24588	-3.67902	-0.00002
H	4.03666	-2.42195	-0.00014
C	7.93551	-2.44920	-0.00001
C	5.11343	2.44712	-0.00009
H	9.02103	-2.45767	0.00003
C	5.78103	3.68389	-0.00005
H	4.02808	2.43620	-0.00012
C	7.92682	2.47722	0.00000
C	7.23285	3.70459	-0.00000
H	9.01231	2.48951	0.00004
C	5.09500	-4.87041	-0.00007
H	4.01249	-4.84855	-0.00011
C	-4.67241	3.20599	-0.00008
C	-6.09420	3.15646	-0.00005
H	-4.12151	2.27063	-0.00011
C	-6.10677	5.62627	-0.00000
C	-6.83709	4.40217	-0.00002
H	-6.66116	6.55967	0.00003
C	7.26168	1.24457	-0.00003
C	7.94313	0.01403	-0.00001
C	5.80392	1.23587	-0.00008
C	7.26602	-1.21892	-0.00004
H	9.02861	0.01594	0.00002
C	5.12714	0.00906	-0.00011
C	5.80824	-1.21535	-0.00008
H	4.04184	0.00715	-0.00014
C	-2.57336	6.90469	-0.00002
C	-3.98698	6.86923	-0.00000
C	-1.84489	5.63113	-0.00006
C	-4.71857	5.66388	-0.00002
H	-4.53040	7.80881	0.00003
C	-2.56965	4.43160	-0.00009
C	-3.97892	4.39775	-0.00007
H	-2.02655	3.49199	-0.00012
C	-1.82488	-5.63759	-0.00008
C	-2.55387	-4.44062	-0.00012

C	-2.54889	-6.91370	-0.00001
C	-3.96326	-4.41173	-0.00008
H	-2.01409	-3.49910	-0.00017
C	-3.96262	-6.88321	0.00002
H	-4.50272	-7.82471	0.00008
C	-0.43956	-5.64352	-0.00010
H	0.09354	-4.69796	-0.00016
C	-4.69846	-5.68046	-0.00001

T7 unrestricted (S=3)

C	-4.87557	2.84894	-0.00002
C	-5.43952	4.12662	-0.00001
C	-6.88934	4.26556	0.00000
C	-7.67570	3.10858	0.00000
C	-4.64036	5.27499	-0.00001
C	-7.44062	5.56469	0.00001
C	-6.64837	6.71197	0.00001
C	-5.19665	6.55292	-0.00000
C	-4.47781	7.74733	0.00000
C	-5.08822	9.02364	0.00001
C	-6.46758	9.18816	0.00002
C	-7.22038	8.01682	0.00002
H	-3.56419	5.15899	-0.00002
H	-3.79465	2.75043	-0.00002
H	-8.75663	3.20873	0.00001
H	-8.52125	5.67109	0.00001
H	-6.94587	10.15865	0.00003
H	-8.30327	8.08401	0.00002
C	-5.44037	-4.44531	-0.00001
C	-6.19802	-5.61503	-0.00000
H	-4.35968	-4.50662	-0.00002
C	-8.25030	-4.27330	0.00001
C	-5.68441	-6.91109	0.00000
C	-7.65646	-5.53453	0.00001
H	-9.33377	-4.20119	0.00001
C	-6.49551	-8.07022	0.00001
C	-8.43410	-6.72812	0.00001
C	-7.88290	-8.00687	0.00002
H	-9.51342	-6.61753	0.00002
H	-8.51394	-8.88576	0.00002
C	-3.14315	8.37778	0.00000
C	-1.76389	8.17447	-0.00000
C	-3.74140	9.65988	0.00001
C	-1.12982	6.93325	-0.00001
C	-0.96503	9.39705	0.00001
C	-2.99265	10.82984	0.00002
H	-1.72361	6.02826	-0.00002
C	0.42428	9.28062	0.00001
C	-1.60971	10.66754	0.00002
H	-3.43859	11.81563	0.00003
H	1.02828	10.18299	0.00001
H	-0.97388	11.54669	0.00002

C	8.53954	3.66131	0.00001
C	8.27377	1.22376	-0.00000
C	9.13722	2.40187	0.00001
H	9.17160	4.54428	0.00001
C	8.94909	0.00421	-0.00000
C	10.55310	2.24495	0.00001
C	10.35952	-0.10503	0.00001
H	11.15288	3.14908	0.00002
C	11.19128	1.00732	0.00002
H	12.27096	0.93693	0.00002
C	-5.27038	-8.91827	0.00001
C	-4.72293	-10.19499	0.00002
C	-4.47091	-7.75148	0.00000
C	-3.33234	-10.26099	0.00002
H	-5.32387	-11.09472	0.00003
C	-3.07681	-7.77607	-0.00000
C	-2.48841	-9.11299	0.00001
H	-2.84892	-11.23233	0.00002
C	-2.24852	-6.65552	-0.00001
C	-1.09908	-9.22537	0.00001
C	-0.85405	-6.77312	-0.00001
H	-2.68581	-5.66533	-0.00002
C	-0.24942	-8.09824	0.00000
H	-0.65052	-10.21428	0.00002
C	6.57026	-2.48815	-0.00001
C	7.82587	-5.00782	0.00001
C	7.96181	-2.55962	-0.00000
H	6.08287	-1.52163	-0.00002
C	8.62118	-3.86301	0.00001
H	8.30504	-5.98225	0.00001
C	8.82793	-1.46689	-0.00000
C	10.04393	-3.93983	0.00002
H	10.48744	-4.93003	0.00002
C	10.87583	-2.82343	0.00002
H	11.95250	-2.93037	0.00002
C	10.23694	-1.58998	0.00001
C	6.41563	-4.94867	0.00000
C	5.60938	-6.09156	0.00000
C	5.77575	-3.64022	-0.00001
H	6.08273	-7.06848	0.00001
C	1.14538	-8.20101	0.00000
H	1.59952	-9.18701	0.00001
C	-0.02964	-5.64603	-0.00002
H	-0.48428	-4.66042	-0.00002
C	6.29368	2.64690	-0.00001
C	4.90520	2.79714	-0.00002
C	7.13871	3.83333	-0.00000
H	4.27923	1.91042	-0.00002
C	6.52993	5.09254	0.00000
C	0.89401	5.57454	-0.00002
H	7.15653	5.97901	0.00001
C	0.26480	6.82143	-0.00001
H	0.28390	4.67684	-0.00002

C	2.47092	7.90297	0.00000
C	1.07786	8.02989	0.00000
H	3.07980	8.80169	0.00001
C	6.88900	1.38072	-0.00001
H	6.25041	0.50670	-0.00002
C	-5.27567	-2.01333	-0.00002
C	-6.04087	-3.18160	-0.00001
H	-4.19315	-2.09246	-0.00002
C	-8.08067	-1.81199	0.00000
C	-7.49404	-3.08167	-0.00000
H	-9.16338	-1.73349	0.00001
C	3.11139	6.65019	-0.00000
C	4.50697	6.50725	0.00000
C	2.28654	5.44736	-0.00001
C	5.13170	5.25136	-0.00000
H	5.12465	7.39982	0.00001
C	2.90572	4.19467	-0.00002
C	4.29620	4.05589	-0.00001
H	2.28779	3.30252	-0.00002
C	-7.11434	1.81838	-0.00000
C	-7.88977	0.64922	0.00000
C	-5.66133	1.69231	-0.00001
C	-7.31588	-0.63071	-0.00000
H	-8.97154	0.73853	0.00001
C	-5.08641	0.41873	-0.00002
C	-5.86178	-0.74377	-0.00001
H	-4.00480	0.32991	-0.00003
C	3.57500	-4.70398	-0.00001
C	2.18064	-4.61357	-0.00002
C	4.20395	-6.01973	-0.00000
C	1.36509	-5.74826	-0.00001
H	1.71700	-3.63233	-0.00002
C	3.38234	-7.15682	0.00000
H	3.84605	-8.13823	0.00001
C	4.38163	-3.56150	-0.00002
H	3.90890	-2.58445	-0.00002
C	1.98227	-7.06957	-0.00000