Supporting Information

Part I Excitation energies

Table I. Vertical (relaxed) excitation energies in eV for *trans*-polyacetylenes $C_{2n}H_{2n+2}$. Calculated by DMRG-CI at M = 1000* using energy-ordered active spaces (*n*e, *n*o), where 2^1A_g is the first dark state, 1^1B_u is the first bright state.

	$C_{10}H_{12}$	$C_{12}H_{14}$	$C_{14}H_{16}$	$C_{16}H_{18}$	$C_{18}H_{20}$	$C_{20}H_{22}$
1^1A_g-2^1A_g	5.43 (4.01)	4.76 (3.41)	4.64 (3.22)	4.23 (2.86)	4.08 (2.76)	3.92 (2.53)
1^1A_g-1^1B_u	5.35 (4.98)	4.94 (4.60)	4.66 (4.29)	4.42 (4.07)	4.24 (3.87)	4.10 (3.74)

*The relaxed 1^1B_u energy for $C_{20}H_{22}$ was computed at M = 500.

Table II. Vertical (relaxed)* excitation energies in eV for *trans*-polyacetylenes $C_{2n}H_{2n+2}$. Calculated by DMRG-CI at M = 1000 using single-π active spaces (*n*e, *n*o), where 2^1A_g is the first dark state, 1^1B_u is the second dark state, 2^1B_u is the first bright state.

	$C_{10}H_{12}$	$C_{12}H_{14}$	$C_{14}H_{16}$	$C_{16}H_{18}$	$C_{18}H_{20}$	$C_{20}H_{22}$
1^1A_g-2^1A_g	4.51 (3.36)	4.15 (2.99)	3.91 (2.73)	3.80 (2.58)	3.76 (2.51)	3.79 (2.52)
1^1A_g-1^1B_u	5.54	5.11	4.72	4.54	4.35	4.55
1^1A_g-2^1B_u	5.77 (5.49)	5.41 (5.13)	5.16 (4.87)	4.98 (4.68)	4.83 (4.54)	4.72 (4.41)

* Vertical excitation energies only for 1^1A_g-1^1B_u .

Table III. Experimental excitation energies in eV for *trans*-polyacetylenes $C_{2n}H_{2n+2}$. By B. E. Kohler [*J. Chem. Phys.* **1988**, 88, 2788].

	$C_{10}H_{12}$	$C_{12}H_{14}$	$C_{14}H_{16}$
1^1A_g-2^1A_g	3.03	2.69	2.44
1^1A_g-1^1B_u	3.57	3.31	3.12

Part II DMRG-CI optimized bond lengths

Table I. Ground state relaxed bond lengths of *trans*-polyacetylenes $C_{2n}H_{2n+2}$ with M = 100, 500, and 1000, using single-π active spaces (*n*e, *n*o).

	M	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10	C10-C11
$C_{10}H_{12}$	100	1.3498	1.4580	1.3579	1.4522	1.3592					
	500	1.3501	1.4577	1.3582	1.4519	1.3596					
	1000	1.3501	1.4577	1.3582	1.4519	1.3596					
$C_{12}H_{14}$	100	1.3489	1.4583	1.3569	1.4518	1.3588	1.4505				
	500	1.3502	1.4573	1.3585	1.4509	1.3603	1.4496				
	1000	1.3502	1.4573	1.3585	1.4508	1.3604	1.4496				
$C_{14}H_{16}$	100	1.3477	1.4593	1.3555	1.4529	1.3575	1.4511	1.3582			
	500	1.3499	1.4580	1.3584	1.4516	1.3602	1.4501	1.3606			
	1000	1.3501	1.4575	1.3586	1.4509	1.3606	1.4494	1.3611			
$C_{16}H_{18}$	100	1.3467	1.4604	1.3536	1.4542	1.3557	1.4521	1.3565	1.4514		
	500	1.3494	1.4582	1.3577	1.4518	1.3597	1.4501	1.3604	1.4497		
	1000	1.3499	1.4579	1.3582	1.4515	1.3603	1.4498	1.3609	1.4494		
$C_{18}H_{20}$	100	1.3453	1.4597	1.3521	1.4542	1.3539	1.4519	1.3552	1.4514	1.3554	
	500	1.3487	1.4586	1.3569	1.4524	1.3589	1.4505	1.3595	1.4498	1.3598	
	1000	1.3495	1.4583	1.3579	1.4520	1.3599	1.4499	1.3605	1.4492	1.3608	
$C_{20}H_{22}$	100	1.3437	1.4601	1.3509	1.4541	1.3526	1.4523	1.3532	1.4514	1.3541	1.4510
	500	1.3477	1.4587	1.3558	1.4522	1.3580	1.4501	1.3590	1.4491	1.3594	1.4489
	1000	1.3490	1.4583	1.3571	1.4519	1.3591	1.4499	1.3600	1.4491	1.3603	1.4489

Table II. Optimized S_1 (first dark state) bond lengths *trans*-polyacetylenes $C_{2n}H_{2n+2}$ with M = 100, 500, and 1000, using single-π active spaces (*n*e, *n*o).

	M	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10	C10-C11
$C_{10}H_{12}$	100	1.4145	1.3851	1.4477	1.3850	1.4338					
	500	1.4168	1.3869	1.4479	1.3877	1.4337					
	1000	1.4160	1.3874	1.4474	1.3876	1.4334					
$C_{12}H_{14}$	100	1.3889	1.3968	1.4408	1.3766	1.4321	1.3858				
	500	1.3978	1.3973	1.4415	1.3821	1.4326	1.3908				
	1000	1.3994	1.3963	1.4425	1.3822	1.4327	1.3911				
$C_{14}H_{16}$	100	1.3692	1.4120	1.4288	1.3737	1.4362	1.3806	1.4252			
	500	1.3836	1.4070	1.4325	1.3794	1.4341	1.3868	1.4248			
	1000	1.3855	1.4071	1.4325	1.3811	1.4344	1.3883	1.4258			
$C_{16}H_{18}$	100	1.3562	1.4285	1.4086	1.3796	1.4359	1.3741	1.4251	1.3820		
	500	1.3706	1.4189	1.4193	1.3816	1.4348	1.3813	1.4250	1.3880		
	1000	1.3745	1.4167	1.4216	1.3826	1.4346	1.3833	1.4255	1.3895		
$C_{18}H_{20}$	100	1.3463	1.4448	1.3847	1.3960	1.4291	1.3703	1.4317	1.3782	1.4212	
	500	1.3597	1.4313	1.4031	1.3889	1.4309	1.3770	1.4285	1.3840	1.4218	
	1000	1.3645	1.4278	1.4077	1.3885	1.4315	1.3795	1.4277	1.3867	1.4213	
$C_{20}H_{22}$	100	1.3426	1.4523	1.3699	1.4114	1.4145	1.3728	1.4359	1.3706	1.4247	1.3779
	500	1.3519	1.4413	1.3880	1.3996	1.4229	1.3763	1.4313	1.3781	1.4233	1.3832
	1000	1.3568	1.4372	1.3941	1.3968	1.4255	1.378	1.4302	1.3820	1.4214	1.3874

Table III. Optimized S_3 (first bright state) bond lengths *trans*-polyacetylenes $C_{2n}H_{2n+2}$ with M = 100, 500, and 1000, using single-π active spaces (*n*e, *n*o).

	M	C1-C2	C2-C3	C3-C4	C4-C5	C5-C6	C6-C7	C7-C8	C8-C9	C9-C10	C10-C11
$C_{10}H_{12}$	100	1.3680	1.4235	1.3927	1.3989	1.4032					
	500	1.3691	1.4234	1.3945	1.4002	1.4034					
	1000	1.3691	1.4237	1.3943	1.4007	1.4031					
$C_{12}H_{14}$	100	1.3639	1.4299	1.3872	1.4057	1.3999	1.3976				
	500	1.3642	1.4303	1.3871	1.4063	1.3984	1.3989				
	1000	1.3646	1.4298	1.3877	1.4056	1.3993	1.3980				
$C_{14}H_{16}$	100	1.3588	1.4365	1.3804	1.4112	1.3940	1.3988	1.399			
	500	1.3609	1.4352	1.3824	1.4112	1.3949	1.3995	1.3989			
	1000	1.3610	1.4351	1.3818	1.4115	1.3944	1.4000	1.3986			
$C_{16}H_{18}$	100	1.3548	1.4418	1.3735	1.4173	1.3868	1.4019	1.3953	1.3973		
	500	1.3568	1.4404	1.3759	1.4174	1.3888	1.4039	1.3963	1.3976		
	1000	1.3583	1.4394	1.3777	1.4165	1.3901	1.4032	1.3967	1.3988		
$C_{18}H_{20}$	100	1.3516	1.4461	1.3681	1.4236	1.3809	1.4068	1.3914	1.3988	1.3956	
	500	1.3548	1.4436	1.3721	1.4223	1.3845	1.4087	1.3926	1.4010	1.3953	
	1000	1.3559	1.4431	1.3736	1.4214	1.3858	1.4070	1.3938	1.3997	1.3966	
$C_{20}H_{22}$	100	1.3495	1.4493	1.3637	1.4291	1.3755	1.4121	1.3865	1.4014	1.3931	1.3973
	500	1.3522	1.4475	1.3687	1.4264	1.3807	1.4121	1.3903	1.4027	1.3964	1.3981
	1000	1.3528	1.4473	1.3689	1.4265	1.3805	1.4125	1.3895	1.4027	1.3955	1.3981

Part III DMRG-CI optimized *trans*-polyacetylene geometries using energy-ordered active spaces at M = 1000 (unless otherwise stated), in XYZ and Angstrom

$C_{10}H_{12}$, S_0

C	-5.522514	-0.214735	0.000000
H	-5.598308	-1.295874	0.000000
H	-6.448819	0.344004	0.000000
C	-4.338994	0.402051	0.000000
H	-4.311433	1.487283	0.000000
C	-3.060118	-0.277019	-0.000000
H	-3.079425	-1.362325	-0.000000
C	-1.873410	0.359347	-0.000000
H	-1.857428	1.444633	-0.000000
C	-0.591716	-0.315465	-0.000000
H	-0.609149	-1.400987	-0.000000
C	0.591719	0.315453	-0.000000
H	0.609152	1.400975	-0.000000
C	1.873413	-0.359359	-0.000000
H	1.857431	-1.444645	-0.000000
C	3.060120	0.277008	-0.000000
H	3.079427	1.362313	-0.000000
C	4.338997	-0.402062	0.000000
H	4.311438	-1.487294	0.000000
C	5.522517	0.214723	0.000000
H	5.598314	1.295863	0.000000
H	6.448821	-0.344018	0.000000

$C_{10}H_{12}$, S_1

C	-5.555776	-0.205736	0.000000
H	-5.678085	-1.281673	0.000000
H	-6.451585	0.398561	0.000000
C	-4.323499	0.367413	0.000000
H	-4.271135	1.452359	0.000000
C	-3.088410	-0.322172	0.000000
H	-3.110530	-1.406636	0.000000
C	-1.853746	0.319529	-0.000000
H	-1.850832	1.405167	-0.000000
C	-0.617284	-0.327548	-0.000000
H	-0.612930	-1.412844	-0.000000
C	0.617287	0.327536	-0.000000
H	0.612934	1.412832	-0.000000
C	1.853749	-0.319541	-0.000000
H	1.850835	-1.405178	-0.000000
C	3.088413	0.322160	-0.000000
H	3.110533	1.406624	0.000000
C	4.323502	-0.367425	-0.000000
H	4.271138	-1.452371	-0.000000
C	5.555779	0.205724	0.000000
H	5.678089	1.281661	0.000000
H	6.451588	-0.398573	0.000000

$C_{10}H_{12}$, S_2

C	-5.570245	-0.243251	0.000016
H	-5.655780	-1.321564	0.000115
H	-6.481612	0.335825	-0.000046
C	-4.314611	0.383492	-0.000035
H	-4.300855	1.469437	-0.000141

C	-3.118434	-0.268502	0.000029
H	-3.119745	-1.353956	0.000094
C	-1.828161	0.385232	0.000001
H	-1.811945	1.469307	-0.000073
C	-0.635257	-0.300893	0.000020
H	-0.671223	-1.386149	0.000007
C	0.635251	0.300316	0.000025
H	0.671158	1.385576	0.000027
C	1.828231	-0.385702	0.000001
H	1.812159	-1.469775	-0.000078
C	3.118354	0.268301	0.000032
H	3.119397	1.353756	0.000104
C	4.314716	-0.383333	-0.000033
H	4.301360	-1.469279	-0.000132
C	5.570175	0.243845	0.000011
H	5.655396	1.322188	0.000105
H	6.481708	-0.335001	-0.000049

$C_{12}H_{14}$, S_0

C	-6.759567	-0.205803	-0.000068
H	-6.833324	-1.286691	-0.000087
H	-7.685266	0.349917	-0.000034
C	-5.568663	0.412041	-0.000002
H	-5.535755	1.496648	0.000115
C	-4.295657	-0.273189	-0.000009
H	-4.322712	-1.359172	-0.000054
C	-3.105133	0.350048	0.000034
H	-3.083548	1.435921	0.000003
C	-1.826765	-0.327704	0.000036
H	-1.843294	-1.412987	-0.000090
C	-0.638461	0.309271	0.000082
H	-0.628252	1.395042	0.000073
C	0.639109	-0.352699	0.000082
H	0.632009	-1.438294	0.000067
C	1.823778	0.291071	0.000042
H	1.831018	1.376694	-0.000080
C	3.109701	-0.372595	0.000039
H	3.103200	-1.458240	0.000009
C	4.288831	0.272545	-0.000008
H	4.295345	1.358309	-0.000058
C	5.576300	-0.387259	-0.000001
H	5.568993	-1.472554	0.000121
C	6.754763	0.254388	-0.000071
H	6.812613	1.337194	-0.000092
H	7.690704	-0.291736	-0.000029

$C_{12}H_{14}$, S_1

C	-6.800863	-0.240745	-0.000221
H	-6.892076	-1.318769	-0.000644
H	-7.710658	0.340968	-0.000232
C	-5.549006	0.377102	0.000173
H	-5.525789	1.462688	0.000626
C	-4.346854	-0.287422	0.000132
H	-4.358077	-1.372834	0.000150
C	-3.070501	0.354721	0.000218
H	-3.058214	1.439776	0.000414
C	-1.870327	-0.315838	0.000246

H	-1.882653	-1.400912	0.000700
C	-0.601678	0.326316	-0.000105
H	-0.595267	1.411989	-0.000394
C	0.601676	-0.327802	0.000044
H	0.595358	-1.413465	0.000530
C	1.870190	0.314613	-0.000438
H	1.882162	1.399706	-0.000989
C	3.070633	-0.355463	-0.000289
H	3.058858	-1.440512	-0.000324
C	4.346612	0.287444	-0.000200
H	4.357119	1.372842	-0.000362
C	5.549251	-0.376254	-0.000078
H	5.526930	-1.461865	-0.000558
C	6.800736	0.242407	0.000376
H	6.891449	1.320561	0.000755
H	7.710957	-0.339087	0.000490

$C_{12}H_{14}$, S_2

C	-6.782098	-0.210342	0.000099
H	-6.889830	-1.287814	0.000278
H	-7.686968	0.379795	-0.000005
C	-5.557796	0.380146	-0.000026
H	-5.511215	1.464843	-0.000249
C	-4.316384	-0.309315	0.000065
H	-4.344193	-1.394360	0.000184
C	-3.087107	0.316456	-0.000040
H	-3.074508	1.402411	-0.000223
C	-1.849878	-0.340129	0.000011
H	-1.850094	-1.425266	0.000026
C	-0.618204	0.314481	-0.000020
H	-0.625227	1.400148	-0.000099
C	0.618234	-0.321628	-0.000024
H	0.625792	-1.407259	-0.000118
C	1.849309	0.334098	0.000018
H	1.848037	1.419277	0.000048
C	3.087732	-0.320235	-0.000037
H	3.077645	-1.406145	-0.000216
C	4.315148	0.309352	0.000064
H	4.339652	1.394369	0.000185
C	5.558978	-0.376010	-0.000024
H	5.516758	-1.460917	-0.000222
C	6.781440	0.218424	0.000089
H	6.886689	1.296389	0.000258
H	7.688053	-0.370603	-0.000000

$C_{14}H_{16}$, S_0

C	-7.987133	-0.237710	0.000026
H	-8.055185	-1.319332	0.000152
H	-8.917252	0.314811	-0.000033
C	-6.805848	0.388701	-0.000050
H	-6.786535	1.474050	-0.000144
C	-5.523749	-0.280706	0.000015
H	-5.535754	-1.366201	0.000153
C	-4.340898	0.361848	-0.000052
H	-4.331713	1.447276	-0.000107
C	-3.055834	-0.304653	-0.000005
H	-3.065201	-1.390178	0.000102

C	-1.874524	0.336030	-0.000041
H	-1.867583	1.421776	-0.000038
C	-0.591915	-0.323900	-0.000024
H	-0.595696	-1.409254	0.000033
C	0.591990	0.326398	-0.000022
H	0.595924	1.411733	0.000035
C	1.874427	-0.333867	-0.000038
H	1.867072	-1.419630	-0.000041
C	3.056045	0.306242	0.000002
H	3.066059	1.391746	0.000109
C	4.340640	-0.361144	-0.000044
H	4.330628	-1.446583	-0.000098
C	5.524104	0.280246	0.000019
H	5.537106	1.365759	0.000147
C	6.805448	-0.390468	-0.000046
H	6.784875	-1.475821	-0.000141
C	7.987373	0.234674	0.000026
H	8.056401	1.316117	0.000144
H	8.916798	-0.318455	-0.000033

$C_{14}H_{16}$, S_1

C	-8.020458	-0.240343	-0.000014
H	-8.117768	-1.318529	-0.000024
H	-8.929783	0.343648	-0.000024
C	-6.786293	0.363936	0.000006
H	-6.756118	1.449653	0.000022
C	-5.573205	-0.305948	0.000032
H	-5.582858	-1.390637	0.000082
C	-4.303402	0.347706	0.000020
H	-4.299920	1.432844	-0.000012
C	-3.101570	-0.311809	0.000077
H	-3.108288	-1.397249	0.000232
C	-1.836895	0.331261	-0.000042
H	-1.831574	1.416853	-0.000182
C	-0.631609	-0.323515	0.000014
H	-0.633214	-1.408785	0.000098
C	0.631723	0.329916	-0.000062
H	0.633725	1.415160	-0.000161
C	1.836576	-0.325700	-0.000055
H	1.830140	-1.411311	-0.000104
C	3.102049	0.315759	-0.000025
H	3.110407	1.401172	-0.000005
C	4.302693	-0.345867	-0.000053
H	4.297116	-1.431020	-0.000154
C	5.574045	0.304736	0.000029
H	5.586001	1.389426	0.000106
C	6.785389	-0.368183	0.000003
H	6.752131	-1.453869	-0.000077
C	8.021106	0.232743	0.000074
H	8.121019	1.310544	0.000155
H	8.928904	-0.353088	0.000051

$C_{14}H_{16}$, S_2

C	-8.005995	-0.211970	0.000002
H	-8.115824	-1.289723	-0.000125
H	-8.911158	0.379692	0.000101
C	-6.788226	0.374134	0.000054

H	-6.740651	1.458964	0.000236
C	-5.542950	-0.316938	-0.000053
H	-5.570797	-1.401700	-0.000123
C	-4.319559	0.312388	-0.000002
H	-4.306361	1.398107	0.000174
C	-3.078259	-0.347039	-0.000071
H	-3.080722	-1.432229	-0.000082
C	-1.852478	0.303939	-0.000051
H	-1.859580	1.389757	0.000046
C	-0.612849	-0.331099	-0.000078
H	-0.599062	-1.416325	-0.000055
C	0.613063	0.337611	-0.000071
H	0.599676	1.422803	-0.000023
C	1.852266	-0.298275	-0.000058
H	1.858229	-1.384140	0.000035
C	3.078857	0.351157	-0.000071
H	3.082964	1.436314	-0.000059
C	4.318973	-0.310457	-0.000004
H	4.303680	-1.396185	0.000197
C	5.543933	0.315755	-0.000062
H	5.574016	1.400521	-0.000127
C	6.787225	-0.378559	0.000055
H	6.736244	-1.463329	0.000271
C	8.006540	0.204080	-0.000006
H	8.118913	1.281263	-0.000149
H	8.909963	-0.389011	0.000107

$C_{16}H_{18}$, S_0

C	-9.223720	-0.225456	0.000218
H	-9.291103	-1.306792	0.000513
H	-10.153280	0.325909	-0.000207
C	-8.037066	0.402132	0.000010
H	-8.013676	1.487035	-0.000354
C	-6.758394	-0.273919	0.000138
H	-6.777393	-1.359710	0.000476
C	-5.572245	0.357535	-0.000132
H	-5.556937	1.443230	-0.000402
C	-4.290994	-0.313160	-0.000055
H	-4.301702	-1.398411	-0.000165
C	-3.104638	0.330359	0.000011
H	-3.098164	1.416005	0.000087
C	-1.826337	-0.328746	-0.000046
H	-1.832332	-1.414423	-0.000181
C	-0.641184	0.314905	0.000025
H	-0.634447	1.400484	0.000032
C	0.641403	-0.347269	-0.000053
H	0.635904	-1.432761	-0.000377
C	1.825047	0.299113	0.000084
H	1.827196	1.384893	0.000168
C	3.106473	-0.353929	0.000024
H	3.106419	-1.439514	-0.000039
C	4.288338	0.297879	-0.000002
H	4.290225	1.383272	-0.000180
C	5.575749	-0.361024	0.000008
H	5.571654	-1.446669	-0.000161
C	6.754389	0.284601	0.000101
H	6.760204	1.370340	0.000086

C	8.041863	-0.375166	0.000152
H	8.034014	-1.460358	0.000253
C	9.220763	0.267157	0.000064
H	9.277357	1.349507	-0.000041
H	10.156595	-0.276600	0.000015

$C_{16}H_{18}$, S_1

C	-9.251603	-0.229053	0.000370
H	-9.348473	-1.307147	0.000999
H	-10.161126	0.353497	0.000261
C	-8.018654	0.375103	-0.000205
H	-7.984842	1.460476	-0.000831
C	-6.799575	-0.301143	-0.000109
H	-6.817146	-1.386204	-0.000025
C	-5.540766	0.336829	-0.000328
H	-5.530174	1.422388	-0.000560
C	-4.335788	-0.326478	-0.000512
H	-4.339966	-1.411429	-0.001145
C	-3.068708	0.327545	-0.000092
H	-3.070130	1.413085	0.000506
C	-1.864499	-0.320752	-0.000463
H	-1.866174	-1.406608	-0.001278
C	-0.605590	0.324526	0.000307
H	-0.597325	1.409700	0.001379
C	0.605734	-0.340708	0.000048
H	0.598101	-1.425835	-0.000140
C	1.863866	0.306012	0.000394
H	1.863630	1.391921	0.000974
C	3.069617	-0.339424	0.000431
H	3.074292	-1.424911	0.000963
C	4.334441	0.319027	0.000153
H	4.334260	1.404036	-0.000063
C	5.542440	-0.338777	0.000332
H	5.537390	-1.424302	0.000939
C	6.797484	0.306760	-0.000159
H	6.808662	1.391792	-0.000672
C	8.020947	-0.361881	-0.000016
H	7.994801	-1.447462	0.000489
C	9.250198	0.249936	-0.000491
H	9.341470	1.328828	-0.001024
H	10.163186	-0.328897	-0.000364

$C_{16}H_{18}$, S_2

C	-9.235607	-0.210174	-0.001819
H	-9.332360	-1.288889	-0.003930
H	-10.147772	0.368969	-0.000223
C	-8.022231	0.389964	-0.000099
H	-7.979759	1.474590	0.002797
C	-6.771478	-0.300640	-0.001054
H	-6.801080	-1.385849	-0.002852
C	-5.552967	0.320983	0.000617
H	-5.535560	1.406877	0.002861
C	-4.308666	-0.342909	-0.000041
H	-4.314875	-1.428072	-0.000663
C	-3.084063	0.305027	0.000648
H	-3.085395	1.390793	0.001784
C	-1.846720	-0.338234	0.000493

H	-1.843040	-1.423888	0.000665
C	-0.617726	0.313855	0.000519
H	-0.621992	1.399510	0.000629
C	0.617750	-0.330031	0.000729
H	0.622640	-1.415632	0.001689
C	1.846015	0.323449	0.000117
H	1.840445	1.409140	-0.000552
C	3.084832	-0.316943	0.000614
H	3.089349	-1.402654	0.002063
C	4.307216	0.335195	-0.000325
H	4.309045	1.420425	-0.001428
C	5.554556	-0.322982	0.000409
H	5.542793	-1.408862	0.002346
C	6.769288	0.306191	-0.000883
H	6.792297	1.391423	-0.002458
C	8.024678	-0.376377	-0.000011
H	7.990192	-1.461319	0.002077
C	9.234393	0.231313	-0.001295
H	9.325895	1.310808	-0.003058
H	10.149887	-0.344607	-0.000296

$C_{18}H_{20}$, S_0

C	-10.452562	-0.247752	-0.000011
H	-10.517621	-1.329487	0.000000
H	-11.383920	0.302303	0.000006
C	-9.271415	0.382261	-0.000132
H	-9.254500	1.467571	-0.000278
C	-7.988658	-0.284789	-0.000124
H	-7.999182	-1.370403	-0.000119
C	-6.806646	0.358026	-0.000065
H	-6.798742	1.443540	0.000124
C	-5.521169	-0.306569	-0.000032
H	-5.528299	-1.392036	0.000229
C	-4.339658	0.337480	-0.000025
H	-4.335991	1.423258	0.000046
C	-3.057351	-0.317782	0.000045
H	-3.057943	-1.403210	-0.000105
C	-1.874309	0.334832	0.000136
H	-1.873121	1.420202	0.000033
C	-0.590693	-0.322486	0.000167
H	-0.594442	-1.408174	0.000107
C	0.590710	0.322254	0.000173
H	0.594458	1.407942	0.000130
C	1.874324	-0.335067	0.000129
H	1.873130	-1.420437	0.000003
C	3.057370	0.317540	0.000049
H	3.057970	1.402968	-0.000097
C	4.339671	-0.337733	-0.000027
H	4.335992	-1.423512	0.000023
C	5.521189	0.306302	-0.000029
H	5.528331	1.391769	0.000230
C	6.806659	-0.358308	-0.000062
H	6.798741	-1.443822	0.000125
C	7.988679	0.284494	-0.000126
H	7.999216	1.370107	-0.000138
C	9.271426	-0.382576	-0.000127
H	9.254494	-1.467886	-0.000276

C	10.452585	0.247412	-0.000013
H	10.517675	1.329146	-0.000020
H	11.383928	-0.302669	0.000005

$C_{18}H_{20}$, S_1

C	-10.473726	-0.228155	0.006412
H	-10.576071	-1.306264	0.005433
H	-11.381920	0.357892	0.008558
C	-9.249567	0.366909	0.005072
H	-9.210249	1.452330	0.006262
C	-8.023684	-0.314345	0.002322
H	-8.042664	-1.399022	0.001053
C	-6.772304	0.327396	0.001084
H	-6.763710	1.412947	0.002176
C	-5.563163	-0.333099	-0.001494
H	-5.567152	-1.418173	-0.002790
C	-4.300963	0.318627	-0.002471
H	-4.302701	1.404343	-0.001791
C	-3.097752	-0.327077	-0.004180
H	-3.093197	-1.412530	-0.005062
C	-1.836565	0.331967	-0.004733
H	-1.837903	1.417066	-0.004666
C	-0.626592	-0.321921	-0.005283
H	-0.631085	-1.407562	-0.005604
C	0.626608	0.321697	-0.005338
H	0.631103	1.407338	-0.005790
C	1.836579	-0.332198	-0.004747
H	1.837912	-1.417295	-0.004597
C	3.097769	0.326837	-0.004265
H	3.093224	1.412290	-0.005260
C	4.300976	-0.318879	-0.002537
H	4.302703	-1.404595	-0.001906
C	5.563184	0.332833	-0.001539
H	5.567187	1.417907	-0.002847
C	6.772315	-0.327679	0.001034
H	6.763704	-1.413232	0.002039
C	8.023707	0.314043	0.002337
H	8.042705	1.398722	0.001148
C	9.249579	-0.367233	0.005056
H	9.210241	-1.452656	0.006150
C	10.473748	0.227811	0.006483
H	10.576114	1.305920	0.005622
H	11.381933	-0.358253	0.008614

$C_{18}H_{20}$, S_2

C	-10.460754	-0.207204	-0.000056
H	-10.562303	-1.285808	-0.000122
H	-11.371267	0.375894	-0.000044
C	-9.250121	0.386030	0.000008
H	-9.204657	1.470789	0.000051
C	-7.998736	-0.306920	0.000020
H	-8.029846	-1.391875	-0.000054
C	-6.782597	0.315775	0.000070
H	-6.762987	1.401438	0.000082
C	-5.535749	-0.352945	0.000048
H	-5.545697	-1.438104	-0.000024
C	-4.315823	0.290338	0.000052

H	-4.315923	1.376255	0.000070
C	-3.074478	-0.352760	-0.000010
H	-3.067136	-1.438117	-0.000050
C	-1.851103	0.308025	-0.000013
H	-1.861295	1.393504	0.000046
C	-0.612440	-0.329294	-0.000039
H	-0.602385	-1.414879	-0.000017
C	0.612457	0.329024	-0.000039
H	0.602402	1.414609	-0.000015
C	1.851120	-0.308295	-0.000017
H	1.861311	-1.393774	0.000039
C	3.074496	0.352489	-0.000016
H	3.067155	1.437846	-0.000052
C	4.315840	-0.290611	0.000042
H	4.315938	-1.376527	0.000061
C	5.535767	0.352670	0.000039
H	5.545717	1.437829	-0.000026
C	6.782613	-0.316053	0.000060
H	6.763000	-1.401716	0.000074
C	7.998754	0.306638	0.000014
H	8.029868	1.391593	-0.000057
C	9.250136	-0.386317	0.000003
H	9.204667	-1.471076	0.000034
C	10.460772	0.206912	-0.000052
H	10.562325	1.285516	-0.000110
H	11.371283	-0.376189	-0.000044

$C_{20}H_{22}$, S_0

C	-11.687051	-0.275590	0.000353
H	-11.742987	-1.357840	0.000907
H	-12.623015	0.267100	0.000089
C	-10.507673	0.366981	0.000022
H	-10.499147	1.452075	-0.000167
C	-9.220328	-0.293397	0.000496
H	-9.226162	-1.379168	0.001280
C	-8.041488	0.351556	-0.000342
H	-8.037937	1.437249	-0.001342
C	-6.753868	-0.305814	-0.000124
H	-6.753724	-1.391149	0.000773
C	-5.572539	0.348540	-0.000795
H	-5.574579	1.434071	-0.001489
C	-4.290071	-0.302349	-0.000204
H	-4.290117	-1.388114	0.000768
C	-3.107395	0.345699	-0.000719
H	-3.104544	1.431230	-0.001375
C	-1.823816	-0.312415	-0.000222
H	-1.826045	-1.397900	0.000656
C	-0.639998	0.336887	-0.000438
H	-0.639214	1.422522	-0.000665
C	0.640125	-0.316098	-0.000082
H	0.638892	-1.401781	0.000009
C	1.824649	0.331896	0.000121
H	1.828849	1.417326	0.000217
C	3.106718	-0.329166	0.000152
H	3.100868	-1.414734	-0.000155
C	4.291633	0.314801	0.000490
H	4.296205	1.400505	0.000793

C	5.571018	-0.342102	0.000291
H	5.567378	-1.427670	-0.000418
C	6.756090	0.305419	0.000666
H	6.762823	1.390675	0.000898
C	8.039143	-0.360746	0.000364
H	8.027727	-1.446457	-0.000144
C	9.223111	0.274612	0.000323
H	9.237818	1.360416	0.000281
C	10.504715	-0.396444	0.000032
H	10.486570	-1.481377	-0.000343
C	11.689020	0.236865	-0.000188
H	11.751766	1.318471	-0.000220
H	12.620971	-0.310733	-0.000502

$C_{20}H_{22}$, S_1

C	-11.704782	-0.241396	0.000110
H	-11.798514	-1.320493	-0.000967
H	-12.618090	0.337499	-0.000076
C	-10.486146	0.363816	0.000441
H	-10.453138	1.449129	0.000985
C	-9.249541	-0.313820	-0.000120
H	-9.268428	-1.398790	-0.000531
C	-8.011106	0.322590	-0.000156
H	-8.000416	1.408281	0.000337
C	-6.793210	-0.339082	-0.000454
H	-6.794888	-1.423839	-0.000779
C	-5.535540	0.319884	-0.000218
H	-5.541746	1.405488	0.000207
C	-4.328541	-0.322054	-0.000391
H	-4.323930	-1.407804	-0.000955
C	-3.070907	0.332051	0.000217
H	-3.070064	1.417251	0.000963
C	-1.859008	-0.323944	0.000008
H	-1.860875	-1.409283	-0.000708
C	-0.606282	0.327772	0.000631
H	-0.607931	1.413390	0.001337
C	0.606511	-0.318707	0.000370
H	0.607851	-1.404362	0.000099
C	1.859604	0.332312	0.000448
H	1.862379	1.417610	0.000759
C	3.070712	-0.325090	0.000122
H	3.068326	-1.410335	-0.000000
C	4.329525	0.326796	-0.000072
H	4.327093	1.412520	0.000044
C	5.534974	-0.317993	-0.000368
H	5.538264	-1.403656	-0.000566
C	6.794593	0.337181	-0.000416
H	6.799875	1.421892	-0.000383
C	8.010104	-0.328881	-0.000464
H	7.995034	-1.414574	-0.000760
C	9.251315	0.301842	-0.000249
H	9.275233	1.386804	-0.000045
C	10.484587	-0.381549	-0.000242
H	10.445828	-1.466698	-0.000976
C	11.705789	0.218280	0.000637
H	11.803267	1.296701	0.001533
H	12.616610	-0.362888	0.000696

$C_{20}H_{22}$, S_2, M = 500

C	-11.685433	-0.272190	-0.008145
H	-11.749547	-1.352634	-0.017116
H	-12.614385	0.277440	-0.007142
C	-10.494798	0.364222	-0.001149
H	-10.482575	1.449317	0.006259
C	-9.218929	-0.296240	-0.003820
H	-9.223480	-1.382125	-0.010323
C	-8.022991	0.350834	0.001489
H	-8.024739	1.436533	0.007519
C	-6.758673	-0.295023	-0.000750
H	-6.751191	-1.380664	-0.007281
C	-5.549877	0.364230	0.004289
H	-5.555158	1.449330	0.008723
C	-4.305159	-0.281933	0.003366
H	-4.307014	-1.368033	0.001841
C	-3.079645	0.359588	0.004848
H	-3.071628	1.444899	0.006238
C	-1.848698	-0.302979	0.005132
H	-1.862278	-1.388891	0.007637
C	-0.612501	0.327776	0.003416
H	-0.597784	1.413410	0.002463
C	0.612056	-0.336897	0.004555
H	0.597775	-1.422597	0.008507
C	1.848059	0.294081	0.001461
H	1.861291	1.380041	-0.000303
C	3.079717	-0.367532	0.002580
H	3.073166	-1.452890	0.007244
C	4.304362	0.275453	-0.000614
H	4.305042	1.361804	-0.002299
C	5.550289	-0.368666	0.000108
H	5.557635	-1.453778	0.002700
C	6.758177	0.292141	-0.002017
H	6.749322	1.377776	-0.001603
C	8.023367	-0.352124	-0.002142
H	8.026187	-1.437968	0.000630
C	9.219103	0.295475	-0.003800
H	9.223810	1.380907	-0.004098
C	10.495355	-0.364902	-0.003088
H	10.482780	-1.449887	-0.002823
C	11.685894	0.271782	-0.003928
H	11.749956	1.353703	-0.005199
H	12.617531	-0.278938	-0.003317

Part IV DMRG-CI optimized *trans*-polyacetylene geometries using single-π active spaces at M = 1000, in XYZ and Angstrom

$C_{10}H_{12}$, S_0

C	-5.570819	-0.217743	-0.000000
H	-5.646184	-1.298410	-0.000000
H	-6.495732	0.342247	-0.000000
C	-4.373490	0.405989	0.000000
H	-4.347960	1.490582	0.000000
C	-3.085856	-0.277393	0.000000
H	-3.106017	-1.362443	-0.000000
C	-1.885150	0.357505	0.000000
H	-1.868794	1.442672	0.000000
C	-0.600421	-0.318770	0.000000
H	-0.615607	-1.403834	0.000000
C	0.600423	0.318772	0.000000
H	0.615610	1.403837	-0.000000
C	1.885151	-0.357504	0.000000
H	1.868791	-1.442671	0.000000
C	3.085859	0.277388	-0.000000
H	3.106026	1.362438	-0.000000
C	4.373489	-0.406002	0.000000
H	4.347952	-1.490594	0.000000
C	5.570825	0.217717	-0.000000
H	5.646212	1.298382	-0.000000
H	6.495727	-0.342292	-0.000000

$C_{10}H_{12}$, S_1

C	-5.634772	-0.234469	-0.000000
H	-5.733843	-1.311401	-0.000000
H	-6.538941	0.355501	-0.000000
C	-4.361014	0.384083	-0.000000
H	-4.332914	1.468759	-0.000000
C	-3.149284	-0.291712	0.000000
H	-3.166177	-1.376389	0.000000
C	-1.854530	0.355348	0.000000
H	-1.839461	1.439906	0.000000
C	-0.641826	-0.318941	0.000000
H	-0.659471	-1.403822	0.000000
C	0.641829	0.318935	0.000000
H	0.659476	1.403816	0.000000
C	1.854532	-0.355357	0.000000
H	1.839462	-1.439915	0.000000
C	3.149289	0.291702	0.000000
H	3.166185	1.376380	0.000000
C	4.361015	-0.384096	-0.000000
H	4.332912	-1.468773	-0.000000
C	5.634775	0.234452	-0.000000
H	5.733850	1.311383	-0.000000
H	6.538941	-0.355522	-0.000000

$C_{10}H_{12}$, S_3

C	-5.582528	-0.212820	-0.000000
H	-5.693298	-1.289832	-0.000000
H	-6.485214	0.380894	-0.000000
C	-4.347937	0.378894	-0.000000
H	-4.303496	1.463525	-0.000000

C	-3.101330	-0.308784	0.000000
H	-3.125589	-1.393418	0.000000
C	-1.859994	0.326179	0.000000
H	-1.849830	1.411808	-0.000000
C	-0.620785	-0.326746	0.000000
H	-0.622851	-1.411863	0.000000
C	0.620783	0.326778	0.000000
H	0.622849	1.411896	0.000000
C	1.859989	-0.326148	0.000000
H	1.849811	-1.411778	0.000000
C	3.101338	0.308788	0.000000
H	3.125621	1.393423	0.000000
C	4.347929	-0.378913	-0.000000
H	4.303461	-1.463544	-0.000000
C	5.582543	0.212757	-0.000000
H	5.693355	1.289764	0.000000
H	6.485206	-0.380992	-0.000000

$C_{12}H_{14}$, S_0

C	-6.812757	-0.230392	-0.000448
H	-6.882706	-1.311267	-0.001188
H	-7.740344	0.324730	-0.000439
C	-5.618020	0.398686	0.000206
H	-5.597411	1.483187	0.000745
C	-4.327575	-0.278410	0.000243
H	-4.342561	-1.363389	0.000431
C	-3.129121	0.361317	0.000212
H	-3.118270	1.446408	-0.000240
C	-1.842140	-0.308453	0.000428
H	-1.851588	-1.393416	0.000872
C	-0.643149	0.334181	0.000034
H	-0.634299	1.419198	-0.000726
C	0.643148	-0.334196	0.000351
H	0.634300	-1.419213	0.001123
C	1.842138	0.308440	-0.000011
H	1.851580	1.393403	-0.000694
C	3.129122	-0.361324	0.000031
H	3.118277	-1.446415	-0.000081
C	4.327570	0.278413	-0.000096
H	4.342536	1.363392	0.000016
C	5.618026	-0.398661	-0.000522
H	5.597443	-1.483162	-0.000953
C	6.812749	0.230444	-0.000089
H	6.882670	1.311321	0.001102
H	7.740351	-0.324654	-0.000290

$C_{12}H_{14}$, S_1

C	-6.865640	-0.239031	-0.000025
H	-6.963220	-1.316481	0.000079
H	-7.771610	0.348758	-0.000048
C	-5.608258	0.375168	-0.000025
H	-5.581662	1.460028	-0.000030
C	-4.386576	-0.300920	0.000041
H	-4.396654	-1.385401	0.000089
C	-3.100662	0.352667	0.000012
H	-3.096473	1.437513	-0.000088
C	-1.887926	-0.310568	0.000047

H	-1.894735	-1.395629	0.000057
C	-0.609513	0.336165	0.000007
H	-0.599424	1.420920	-0.000051
C	0.609249	-0.334588	0.000003
H	0.598901	-1.419357	0.000044
C	1.887873	0.311649	-0.000026
H	1.894930	1.396753	-0.000059
C	3.100478	-0.351731	-0.000032
H	3.095819	-1.436627	-0.000081
C	4.386820	0.300864	0.000002
H	4.397609	1.385374	0.000067
C	5.608099	-0.375852	-0.000049
H	5.580866	-1.460714	-0.000092
C	6.865928	0.237443	0.000013
H	6.964320	1.314822	0.000165
H	7.771433	-0.351051	0.000001

$C_{12}H_{14}$, S_3

C	-6.817580	-0.213712	0.003738
H	-6.927764	-1.290933	0.004544
H	-7.720754	0.379639	0.004685
C	-5.587870	0.377739	0.000740
H	-5.543824	1.462342	-0.000430
C	-4.336289	-0.313623	-0.000661
H	-4.361626	-1.398315	-0.002032
C	-3.100872	0.318299	-0.001188
H	-3.090493	1.404035	0.000332
C	-1.857159	-0.336518	-0.002167
H	-1.856286	-1.421620	-0.003462
C	-0.621221	0.319651	-0.001828
H	-0.628027	1.405093	-0.000897
C	0.621383	-0.320883	-0.002777
H	0.628331	-1.406313	-0.000828
C	1.857127	0.335622	-0.003910
H	1.855892	1.420711	-0.003232
C	3.100993	-0.318860	-0.002738
H	3.091046	-1.404585	-0.001588
C	4.336121	0.313620	-0.000768
H	4.361027	1.398319	-0.000154
C	5.588027	-0.377188	0.001669
H	5.544547	-1.461806	0.001927
C	6.817396	0.214979	0.003185
H	6.926889	1.292268	0.003030
H	7.720957	-0.377793	0.004831

$C_{14}H_{16}$, S_0

C	-8.054331	-0.239551	-0.000194
H	-8.122186	-1.320851	-0.000220
H	-8.983248	0.314008	-0.000450
C	-6.861277	0.392392	-0.000040
H	-6.843290	1.477316	-0.000304
C	-5.569143	-0.281870	0.000140
H	-5.581682	-1.367181	0.000531
C	-4.372495	0.361379	0.000143
H	-4.364043	1.446820	0.000135
C	-3.083766	-0.305264	-0.000086
H	-3.090664	-1.390556	-0.000627

C	-1.886622	0.341259	0.000245
H	-1.880543	1.426613	0.000933
C	-0.598718	-0.323545	0.000043
H	-0.604501	-1.408876	-0.000255
C	0.598718	0.323562	0.000043
H	0.604505	1.408893	-0.000255
C	1.886621	-0.341243	0.000246
H	1.880539	-1.426597	0.000935
C	3.083770	0.305267	-0.000084
H	3.090678	1.390559	-0.000627
C	4.372493	-0.361385	0.000147
H	4.364031	-1.446827	0.000139
C	5.569152	0.281844	0.000140
H	5.581707	1.367154	0.000530
C	6.861268	-0.392451	-0.000046
H	6.843247	-1.477375	-0.000306
C	8.054348	0.239443	-0.000194
H	8.122266	1.320738	-0.000229
H	8.983232	-0.314173	-0.000429

$C_{14}H_{16}$, S_1

C	-8.096644	-0.237619	0.000066
H	-8.195071	-1.315412	0.000076
H	-9.005256	0.346790	0.000065
C	-6.852545	0.372119	0.000033
H	-6.818406	1.456867	-0.000008
C	-5.621431	-0.309346	0.000018
H	-5.639507	-1.393608	0.000050
C	-4.345240	0.341403	-0.000001
H	-4.337586	1.426582	-0.000005
C	-3.130954	-0.316502	-0.000073
H	-3.136254	-1.401563	-0.000166
C	-1.854797	0.338319	-0.000013
H	-1.848040	1.423132	0.000116
C	-0.634869	-0.324269	-0.000043
H	-0.643706	-1.409309	-0.000120
C	0.634871	0.324248	-0.000044
H	0.643710	1.409288	-0.000121
C	1.854799	-0.338340	-0.000011
H	1.848039	-1.423153	0.000118
C	3.130958	0.316473	-0.000072
H	3.136262	1.401535	-0.000168
C	4.345243	-0.341432	0.000001
H	4.337587	-1.426611	-0.000001
C	5.621437	0.309312	0.000020
H	5.639517	1.393574	0.000051
C	6.852548	-0.372158	0.000032
H	6.818403	-1.456906	-0.000005
C	8.096651	0.237571	0.000067
H	8.195088	1.315364	0.000072
H	9.005257	-0.346847	0.000072

$C_{14}H_{16}$, S_3

C	-8.051182	-0.214415	0.000235
H	-8.156215	-1.292343	0.000264
H	-8.958422	0.373073	0.000391
C	-6.827154	0.380678	0.000134

H	-6.782721	1.465107	0.000279
C	-5.570844	-0.313101	-0.000000
H	-5.599497	-1.397775	-0.000247
C	-4.340757	0.316482	-0.000098
H	-4.326361	1.402159	-0.000134
C	-3.092923	-0.343241	0.000013
H	-3.097195	-1.428328	0.000418
C	-1.860721	0.309394	-0.000293
H	-1.864131	1.395033	-0.000807
C	-0.615945	-0.331225	-0.000171
H	-0.607884	-1.416541	0.000012
C	0.615942	0.331007	-0.000172
H	0.607854	1.416325	0.000010
C	1.860749	-0.309547	-0.000292
H	1.864224	-1.395185	-0.000805
C	3.092904	0.343184	0.000014
H	3.097106	1.428271	0.000416
C	4.340772	-0.316465	-0.000096
H	4.326423	-1.402143	-0.000130
C	5.570845	0.313160	-0.000000
H	5.599480	1.397834	-0.000248
C	6.827154	-0.380617	0.000132
H	6.782712	-1.465047	0.000281
C	8.051192	0.214450	0.000237
H	8.156246	1.292376	0.000261
H	8.958418	-0.373058	0.000400

$C_{16}H_{18}$, S_0

C	-9.295887	-0.245936	-0.000000
H	-9.362933	-1.327149	-0.000000
H	-10.225067	0.307042	-0.000000
C	-8.103869	0.387523	-0.000000
H	-8.087304	1.472278	-0.000000
C	-6.810623	-0.285461	-0.000000
H	-6.821941	-1.370595	-0.000000
C	-5.615516	0.359932	0.000000
H	-5.608256	1.445187	0.000000
C	-4.325306	-0.305127	0.000000
H	-4.330976	-1.390241	0.000000
C	-3.129829	0.343841	0.000000
H	-3.125169	1.429038	0.000000
C	-1.840337	-0.318807	0.000000
H	-1.844518	-1.403957	0.000000
C	-0.644643	0.331131	0.000000
H	-0.640650	1.416290	0.000000
C	0.644640	-0.331093	0.000000
H	0.640638	-1.416252	0.000000
C	1.840337	0.318840	0.000000
H	1.844522	1.403990	0.000000
C	3.129825	-0.343818	0.000000
H	3.125151	-1.429015	0.000000
C	4.325306	0.305140	0.000000
H	4.330986	1.390254	0.000000
C	5.615515	-0.359922	0.000000
H	5.608256	-1.445178	0.000000
C	6.810619	0.285473	-0.000000
H	6.821938	1.370608	-0.000000

C	8.103873	-0.387496	-0.000000
H	8.087334	-1.472251	-0.000000
C	9.295883	0.245981	-0.000000
H	9.362920	1.327194	-0.000000
H	10.225064	-0.306994	-0.000000

$C_{16}H_{18}$, S_1

C	-9.326945	-0.232726	0.000000
H	-9.427065	-1.310673	0.000000
H	-10.235692	0.351971	0.000000
C	-8.092366	0.371567	0.000000
H	-8.054585	1.456246	0.000000
C	-6.853507	-0.315714	0.000000
H	-6.874699	-1.399886	0.000000
C	-5.587109	0.330249	-0.000000
H	-5.579041	1.415653	-0.000000
C	-4.370431	-0.326509	-0.000000
H	-4.372530	-1.411449	-0.000000
C	-3.096367	0.332967	-0.000000
H	-3.095108	1.417917	-0.000000
C	-1.878377	-0.322725	-0.000000
H	-1.881748	-1.407920	-0.000000
C	-0.611245	0.330262	-0.000000
H	-0.606054	1.415234	-0.000000
C	0.611237	-0.330218	-0.000000
H	0.606045	-1.415190	-0.000000
C	1.878373	0.322768	-0.000000
H	1.881747	1.407963	-0.000000
C	3.096362	-0.332930	-0.000000
H	3.095097	-1.417880	-0.000000
C	4.370432	0.326542	-0.000000
H	4.372538	1.411481	-0.000000
C	5.587108	-0.330226	-0.000000
H	5.579034	-1.415629	-0.000000
C	6.853511	0.315732	0.000000
H	6.874708	1.399904	0.000000
C	8.092366	-0.371554	0.000000
H	8.054584	-1.456232	0.000000
C	9.326947	0.232736	0.000000
H	9.427071	1.310683	0.000000
H	10.235692	-0.351964	0.000000

$C_{16}H_{18}$, S_3

C	-9.287488	-0.209394	-0.000000
H	-9.392907	-1.287330	-0.000000
H	-10.194802	0.378137	-0.000000
C	-8.065936	0.384634	-0.000000
H	-8.020410	1.469023	-0.000000
C	-6.806788	-0.312799	-0.000000
H	-6.837503	-1.397427	-0.000000
C	-5.579451	0.312982	0.000000
H	-5.562162	1.398610	0.000000
C	-4.328902	-0.352218	0.000000
H	-4.335455	-1.437265	0.000000
C	-3.099627	0.296749	0.000000
H	-3.102116	1.382394	0.000000
C	-1.852448	-0.346262	0.000000

H	-1.843422	-1.431483	0.000000
C	-0.623288	0.317047	0.000000
H	-0.635827	1.402452	0.000000
C	0.623309	-0.317478	0.000000
H	0.635913	-1.402877	0.000000
C	1.852376	0.345999	0.000000
H	1.843187	1.431221	0.000000
C	3.099686	-0.296779	0.000000
H	3.102360	-1.382423	0.000000
C	4.328840	0.352411	0.000000
H	4.335258	1.437455	-0.000000
C	5.579452	-0.312675	-0.000000
H	5.562207	-1.398307	0.000000
C	6.806807	0.313096	-0.000000
H	6.837570	1.397719	-0.000000
C	8.065902	-0.384450	-0.000000
H	8.020266	-1.468836	-0.000000
C	9.287531	0.209418	-0.000000
H	9.393086	1.287341	-0.000000
H	10.194767	-0.378233	-0.000000

$C_{18}H_{20}$, S_0

C	-10.536825	-0.254949	0.000000
H	-10.601307	-1.336379	0.000000
H	-11.467424	0.295746	0.000000
C	-9.346582	0.381050	0.000000
H	-9.332174	1.465880	0.000000
C	-8.051645	-0.289499	0.000000
H	-8.060639	-1.374682	0.000000
C	-6.858430	0.358706	-0.000000
H	-6.853250	1.443970	-0.000000
C	-5.566809	-0.304596	-0.000000
H	-5.570619	-1.389725	0.000000
C	-4.372977	0.346649	-0.000000
H	-4.370373	1.431879	-0.000000
C	-3.082225	-0.313827	-0.000000
H	-3.084903	-1.399070	-0.000000
C	-1.887591	0.337117	-0.000000
H	-1.885181	1.422389	-0.000000
C	-0.597308	-0.322788	-0.000000
H	-0.599579	-1.408047	-0.000000
C	0.597509	0.328441	-0.000000
H	0.600307	1.413656	-0.000000
C	1.887398	-0.332658	-0.000000
H	1.884544	-1.417869	-0.000000
C	3.082157	0.318452	-0.000000
H	3.085464	1.403624	-0.000000
C	4.372156	-0.343622	-0.000000
H	4.367901	-1.428876	-0.000000
C	5.566978	0.305429	-0.000000
H	5.572114	1.390618	0.000000
C	6.857770	-0.358728	-0.000000
H	6.850769	-1.444095	-0.000000
C	8.052422	0.286143	0.000000
H	8.063684	1.371384	0.000000
C	9.346148	-0.386309	0.000000
H	9.329865	-1.471147	0.000000

C	10.537607	0.247265	0.000000
H	10.604343	1.328560	0.000000
H	11.467028	-0.305384	0.000000

$C_{18}H_{20}$, S_1

C	-10.555667	-0.225083	0.000000
H	-10.656488	-1.303264	0.000000
H	-11.465460	0.358526	0.000000
C	-9.330437	0.375459	-0.000000
H	-9.287878	1.459946	-0.000000
C	-8.082670	-0.318582	0.000000
H	-8.110586	-1.402640	0.000000
C	-6.828077	0.319931	-0.000000
H	-6.814018	1.405455	-0.000000
C	-5.606319	-0.339886	-0.000000
H	-5.611632	-1.424630	0.000000
C	-4.336239	0.320398	-0.000000
H	-4.335221	1.405537	-0.000000
C	-3.119680	-0.330068	-0.000000
H	-3.120631	-1.415282	0.000000
C	-1.853000	0.328680	-0.000000
H	-1.850504	1.413652	-0.000000
C	-0.630934	-0.326714	-0.000000
H	-0.634926	-1.411865	0.000000
C	0.630965	0.327354	-0.000000
H	0.635044	1.412499	0.000000
C	1.852976	-0.328171	-0.000000
H	1.850400	-1.413137	-0.000000
C	3.119699	0.330511	-0.000000
H	3.120764	1.415718	0.000000
C	4.336137	-0.320178	-0.000000
H	4.334853	-1.405319	-0.000000
C	5.606381	0.339786	-0.000000
H	5.611903	1.424537	0.000000
C	6.827993	-0.320236	-0.000000
H	6.813658	-1.405768	-0.000000
C	8.082809	0.317845	0.000000
H	8.111067	1.401901	0.000000
C	9.330367	-0.376510	-0.000000
H	9.287534	-1.460988	-0.000000
C	10.555791	0.223683	0.000000
H	10.656952	1.301831	0.000000
H	11.465394	-0.360222	0.000000

$C_{18}H_{20}$, S_3

C	-10.522347	-0.204244	-0.000000
H	-10.627084	-1.282328	-0.000000
H	-11.430458	0.382256	-0.000000
C	-9.303505	0.389754	-0.000000
H	-9.256939	1.474044	-0.000000
C	-8.041773	-0.310606	-0.000000
H	-8.074897	-1.395193	-0.000000
C	-6.817530	0.312358	0.000000
H	-6.797078	1.397902	0.000000
C	-5.564009	-0.357695	0.000000
H	-5.574160	-1.442714	0.000000
C	-4.337561	0.287423	0.000000

H	-4.336726	1.373085	0.000000
C	-3.088203	-0.359688	0.000000
H	-3.081590	-1.444894	0.000000
C	-1.861259	0.301625	0.000000
H	-1.873212	1.387112	0.000000
C	-0.613454	-0.332563	0.000000
H	-0.598816	-1.417867	0.000000
C	0.613507	0.334631	0.000000
H	0.599100	1.419924	0.000000
C	1.861044	-0.300092	0.000000
H	1.872401	-1.385596	0.000000
C	3.088468	0.360330	0.000000
H	3.082604	1.445540	0.000000
C	4.337360	-0.287695	0.000000
H	4.335829	-1.373353	0.000000
C	5.564174	0.356726	0.000000
H	5.574780	1.441749	0.000000
C	6.817510	-0.313704	-0.000000
H	6.796855	-1.399238	0.000000
C	8.041784	0.309196	-0.000000
H	8.074908	1.393789	-0.000000
C	9.303593	-0.391042	-0.000000
H	9.257150	-1.475336	-0.000000
C	10.522353	0.203131	-0.000000
H	10.626956	1.281228	-0.000000
H	11.430546	-0.383246	-0.000000

$C_{20}H_{22}$, S_0

C	-11.777002	-0.264956	0.000000
H	-11.838826	-1.346690	0.000000
H	-12.709135	0.283328	0.000000
C	-10.588570	0.373284	0.000000
H	-10.576358	1.458319	0.000000
C	-9.292100	-0.294395	0.000000
H	-9.299259	-1.379813	0.000000
C	-8.100331	0.354687	0.000000
H	-8.097152	1.440196	-0.000000
C	-6.807386	-0.305880	0.000000
H	-6.809239	-1.391233	0.000000
C	-5.614864	0.346177	-0.000000
H	-5.613866	1.431609	-0.000000
C	-4.323252	-0.312597	-0.000000
H	-4.324092	-1.397991	-0.000000
C	-3.129932	0.339737	-0.000000
H	-3.129239	1.425156	-0.000000
C	-1.839152	-0.318927	-0.000000
H	-1.840033	-1.404337	-0.000000
C	-0.645214	0.333028	-0.000000
H	-0.644170	1.418440	-0.000000
C	0.645057	-0.326167	-0.000000
H	0.643670	-1.411588	-0.000000
C	1.839395	0.325102	-0.000000
H	1.841129	1.410508	-0.000000
C	3.129491	-0.334960	-0.000000
H	3.127312	-1.420391	-0.000000
C	4.323931	0.315421	-0.000000
H	4.326693	1.400812	-0.000000

C	5.614248	-0.345956	-0.000000
H	5.610823	-1.431395	-0.000000
C	6.808433	0.303145	-0.000000
H	6.813047	1.388490	0.000000
C	8.099575	-0.360992	0.000000
H	8.093201	-1.446493	-0.000000
C	9.293393	0.284374	0.000000
H	9.303945	1.369761	0.000000
C	10.587573	-0.387745	0.000000
H	10.571407	-1.472733	0.000000
C	11.778381	0.246012	0.000000
H	11.844528	1.327487	0.000000
H	12.708325	-0.305984	0.000000

$C_{20}H_{22}$, S_1

C	-11.785239	-0.213053	0.000000
H	-11.888933	-1.291198	0.000000
H	-12.694152	0.372301	0.000000
C	-10.565764	0.381689	0.000000
H	-10.518720	1.465981	0.000000
C	-9.311690	-0.320334	0.000000
H	-9.344469	-1.404379	0.000000
C	-8.067758	0.309077	0.000000
H	-8.050383	1.394699	-0.000000
C	-6.839550	-0.356271	0.000000
H	-6.845035	-1.440868	0.000000
C	-5.575032	0.301885	-0.000000
H	-5.577228	1.387222	-0.000000
C	-4.358655	-0.345672	-0.000000
H	-4.353734	-1.430810	-0.000000
C	-3.091788	0.318044	-0.000000
H	-3.096055	1.403065	-0.000000
C	-1.872110	-0.331777	-0.000000
H	-1.870240	-1.417056	-0.000000
C	-0.611675	0.325317	-0.000000
H	-0.611837	1.410406	-0.000000
C	0.611867	-0.328802	-0.000000
H	0.612005	-1.413893	-0.000000
C	1.872305	0.328235	-0.000000
H	1.870505	1.413512	-0.000000
C	3.091968	-0.321711	-0.000000
H	3.096122	-1.406732	-0.000000
C	4.358881	0.341852	-0.000000
H	4.354086	1.426993	-0.000000
C	5.575155	-0.305850	-0.000000
H	5.577208	-1.391186	-0.000000
C	6.839837	0.352148	0.000000
H	6.845460	1.436746	0.000000
C	8.067847	-0.313318	0.000000
H	8.050325	-1.398937	-0.000000
C	9.312019	0.315949	0.000000
H	9.344949	1.399988	0.000000
C	10.565868	-0.386244	0.000000
H	10.518625	-1.470527	0.000000
C	11.785564	0.208273	0.000000
H	11.889505	1.286390	0.000000
H	12.694332	-0.377301	0.000000

$C_{20}H_{22}$, S_3

C	-11.751305	-0.246312	0.000195
H	-11.830936	-1.326649	-0.000014
H	-12.673442	0.318139	0.000251
C	-10.549547	0.374836	0.000226
H	-10.525193	1.459735	0.000209
C	-9.270118	-0.301817	0.000128
H	-9.284374	-1.386942	0.000005
C	-8.061768	0.341498	0.000115
H	-8.056818	1.427098	0.000195
C	-6.794049	-0.312614	0.000025
H	-6.794534	-1.397988	0.000019
C	-5.577578	0.340052	-0.000029
H	-5.578157	1.425427	-0.000063
C	-4.323785	-0.310395	-0.000111
H	-4.324107	-1.395917	-0.000128
C	-3.095231	0.338826	-0.000167
H	-3.091803	1.424059	-0.000072
C	-1.856035	-0.318496	-0.000211
H	-1.862556	-1.403989	-0.000131
C	-0.616436	0.322459	-0.000225
H	-0.609217	1.407888	-0.000221
C	0.616492	-0.336682	-0.000224
H	0.609298	-1.422145	-0.000220
C	1.856010	0.304463	-0.000210
H	1.861705	1.390039	-0.000131
C	3.096083	-0.351102	-0.000165
H	3.093956	-1.436398	-0.000070
C	4.323878	0.299090	-0.000109
H	4.322555	1.384627	-0.000128
C	5.578966	-0.348449	-0.000027
H	5.582266	-1.433736	-0.000060
C	6.793703	0.307643	0.000026
H	6.791587	1.392900	0.000017
C	8.063063	-0.344064	0.000116
H	8.061227	-1.429534	0.000198
C	9.269199	0.304064	0.000127
H	9.279804	1.389152	0.000002
C	10.550684	-0.368946	0.000226
H	10.529655	-1.453877	0.000211
C	11.750398	0.256215	0.000193
H	11.826408	1.336807	-0.000017
H	12.674442	-0.305125	0.000250