

Supplementary material to: Density functional theory with fractional orbital occupations

Jeng-Da Chai*

*Department of Physics, Center for Theoretical Sciences,
and Center for Quantum Science and Engineering,
National Taiwan University, Taipei 10617, Taiwan*

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References (S2).

Total energies and Cartesian coordinates for the lowest singlet and triplet states of n -acenes ($n = 2$ to 46) by spin-unrestricted TAO-LDA ($\theta = 7$ mHartree)/6-31G* (S3 to S88).

TABLE S1. Reaction energies of 30 chemical reactions (S89).

TABLE S2. Equilibrium geometries in EXTS (S89 to S93).

TABLE S3. Singlet-triplet energy gap of n -acenes by KS-DFT/6-31G* (S93).

TABLE S4. Singlet-triplet energy gap of n -acenes by TAO-LDA/6-31G* (S93 to S94).

TABLE S5. Singlet-triplet energy gap of n -acenes by TAO-LDA/6-31G (S94 to S95).

TABLE S6. Active orbital occupation numbers for the lowest singlet states of acenes (S95).

* Electronic mail: jdchai@phys.ntu.edu.tw.

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Total energies (in Hartree) and Cartesian coordinates (in angstrom) for the lowest singlet and triplet states of *n*-acenes (*n* = 2 to 46) at the level of spin-unrestricted TAO-LDA ($\theta = 7$ mHartree)/6-31G*.

```
2-acene (singlet), E = -382.3212449480
C 2.42398048 -0.70477355 0.00000000
C 2.42398047 0.70477355 0.00000000
C 1.23599344 -1.39775201 0.00000000
C 1.23599343 1.39775201 0.00000000
C 0.00000000 -0.71495553 0.00000000
C 0.00000000 0.71495554 0.00000000
C -1.23599344 -1.39775201 0.00000000
C -1.23599343 1.39775202 0.00000000
C -2.42398047 -0.70477355 0.00000000
C -2.42398047 0.70477356 0.00000000
H 1.22707212 -2.49677029 0.00000000
H 1.22707212 2.49677029 0.00000000
H -1.22707212 -2.49677029 0.00000000
H -1.22707212 2.49677030 0.00000000
H 3.37722463 1.24838306 0.00000000
H 3.37722465 -1.24838307 0.00000000
H -3.37722464 1.24838307 0.00000000
H -3.37722464 -1.24838307 0.00000000
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2-acene (triplet), E = -382.2180209884
C 2.47345093 -0.68473334 0.00000000
C 2.47345104 0.68473333 0.00000000
C 1.23419909 -1.39383337 0.00000000
C 1.23419924 1.39383349 0.00000000
C 0.00000000 -0.71837193 0.00000000
C -0.00000000 0.71837196 0.00000000
C -1.23419917 -1.39383345 0.00000000
C -1.23419917 1.39383343 0.00000000
C -2.47345097 -0.68473339 0.00000000
C -2.47345099 0.68473327 0.00000000
H 1.23202477 -2.49206718 0.00000000
H 1.23202503 2.49206735 0.00000000
H -1.23202489 -2.49206726 0.00000000
H -1.23202490 2.49206727 0.00000000
H 3.41530541 1.24655255 0.00000000
H 3.41530524 -1.24655261 0.00000000
H -3.41530535 1.24655251 0.00000000
H -3.41530528 -1.24655264 0.00000000
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```
3-acene (singlet), E = -534.5626973632
C 4.87112782 -0.70824352 0.00000000
C 4.87112789 0.70824341 0.00000000
C 3.68909893 -1.40166621 0.00000000
C 3.68909905 1.40166621 0.00000000
C 2.44507179 -0.72022074 0.00000000
C 2.44507184 0.72022079 0.00000000
C 1.22590001 -1.39916042 0.00000000
C 1.22590001 1.39916058 0.00000000
C 0.00672822 -0.72022075 0.00000000
C 0.00672818 0.72022080 0.00000000
C -1.23729894 -1.40166618 0.00000000
C -1.23729907 1.40166620 0.00000000
C -2.41932784 -0.70824352 0.00000000
C -2.41932791 0.70824341 0.00000000
H 3.68053801 -2.50053668 0.00000000
H 3.68053817 2.50053672 0.00000000
H 1.22590006 -2.49953292 0.00000000
H 1.22590006 2.49953313 0.00000000
H -1.22873804 -2.50053666 0.00000000
H -1.22873821 2.50053671 0.00000000
H 5.82568925 -1.24940384 0.00000000
H 5.82568938 1.24940367 0.00000000
H -3.37388926 -1.24940385 0.00000000
H -3.37388940 1.24940368 0.00000000
```

```
3-acene (triplet), E = -534.4938298497
C 4.91227840 -0.69182595 0.00000000
C 4.91227836 0.69182592 0.00000000
C 3.69300590 -1.39195515 0.00000000
C 3.69300582 1.39195507 0.00000000
C 2.46797152 -0.71718126 0.00000000
C 2.46797156 0.71718120 0.00000000
C 1.22590004 -1.39587120 0.00000000
C 1.22589996 1.39587120 0.00000000
C -0.01617156 -0.71718119 0.00000000
C -0.01617153 0.71718128 0.00000000
C -1.24120582 -1.39195505 0.00000000
C -1.24120592 1.39195515 0.00000000
```

C	-2.46047836	-0.69182592	0.00000000
C	-2.46047842	0.69182594	0.00000000
H	3.68772648	-2.49072437	0.00000000
H	3.68772639	2.49072425	0.00000000
H	1.22590006	-2.49585138	0.00000000
H	1.22590004	2.49585139	0.00000000
H	-1.23592641	-2.49072423	0.00000000
H	-1.23592653	2.49072435	0.00000000
H	5.85798365	-1.24749726	0.00000000
H	5.85798360	1.24749728	0.00000000
H	-3.40618356	-1.24749731	0.00000000
H	-3.40618367	1.24749727	0.00000000

4-acene (singlet), E = -686.8022969856

C	4.86849527	0.70960485	0.00000000
C	4.86849540	-0.70960454	0.00000000
C	3.68839532	-1.40304795	0.00000000
C	2.44124772	-0.72252508	0.00000000
C	2.44124761	0.72252500	0.00000000
C	3.68839508	1.40304803	0.00000000
C	1.22790726	-1.40160612	0.00000000
C	0.00000000	-0.72406617	0.00000000
C	0.00000000	0.72406597	0.00000000
C	1.22790714	1.40160582	0.00000000
C	-1.22790726	-1.40160612	0.00000000
C	-2.44124772	-0.72252508	0.00000000
C	-2.44124761	0.72252500	0.00000000
C	-1.22790714	1.40160582	0.00000000
C	-3.68839532	-1.40304794	0.00000000
C	-4.86849540	-0.70960454	0.00000000
C	-4.86849527	0.70960485	0.00000000
C	-3.68839508	1.40304803	0.00000000
H	5.82352308	1.24991683	0.00000000
H	5.82352331	-1.24991640	0.00000000
H	3.68033563	-2.50188311	0.00000000
H	3.68033524	2.50188313	0.00000000
H	1.22831614	-2.50181909	0.00000000
H	1.22831600	2.50181871	0.00000000
H	-1.22831614	-2.50181908	0.00000000
H	-1.22831600	2.50181873	0.00000000
H	-3.68033563	-2.50188309	0.00000000
H	-5.82352331	-1.24991640	0.00000000
H	-5.82352308	1.24991683	0.00000000
H	-3.68033524	2.50188313	0.00000000

4-acene (triplet), E = -686.7560608051

C	4.90183926	0.69707562	0.00000000
C	4.90183927	-0.69707562	0.00000000
C	3.69558126	-1.39384213	0.00000000
C	2.46826884	-0.71640447	0.00000000
C	2.46826883	0.71640446	0.00000000
C	3.69558125	1.39384213	0.00000000
C	1.22738211	-1.39651115	0.00000000
C	-0.00000004	-0.72352973	0.00000000
C	-0.00000004	0.72352972	0.00000000
C	1.22738211	1.39651114	0.00000000
C	-1.22738203	-1.39651116	0.00000000
C	-2.46826875	-0.71640451	0.00000000
C	-2.46826875	0.71640452	0.00000000
C	-1.22738203	1.39651115	0.00000000
C	-3.69558133	-1.39384221	0.00000000
C	-4.90183931	-0.69707568	0.00000000
C	-4.90183931	0.69707569	0.00000000
C	-3.69558132	1.39384222	0.00000000
H	5.85045966	1.24803201	0.00000000
H	5.85045969	-1.24803201	0.00000000
H	3.68868555	-2.49271337	0.00000000
H	3.68868554	2.49271337	0.00000000
H	1.22900478	-2.49663800	0.00000000
H	1.22900477	2.49663799	0.00000000
H	-1.22900466	-2.49663802	0.00000000
H	-1.22900465	2.49663801	0.00000000
H	-3.68868565	-2.49271349	0.00000000
H	-5.85045970	-1.24803210	0.00000000
H	-5.85045971	1.24803212	0.00000000
H	-3.68868564	2.49271350	0.00000000

5-acene (singlet), E = -839.0416885908

C	7.31114719	-0.70969377	0.00000000
C	7.31114717	0.70969382	0.00000000
C	6.13089932	-1.40330814	0.00000000
C	6.13089928	1.40330815	0.00000000
C	4.88348555	-0.72321752	0.00000000

C	4.88348554	0.72321750	0.00000000
C	3.67108847	-1.40236559	0.00000000
C	3.67108848	1.40236555	0.00000000
C	2.44037950	-0.72588296	0.00000000
C	2.44037951	0.72588295	0.00000000
C	1.21786109	-1.40357867	0.00000000
C	1.21786110	1.40357862	0.00000000
C	-0.00465730	-0.72588296	0.00000000
C	-0.00465729	0.72588293	0.00000000
C	-1.23536625	-1.40236559	0.00000000
C	-1.23536625	1.40236556	0.00000000
C	-2.44776332	-0.72321750	0.00000000
C	-2.44776331	0.72321751	0.00000000
C	-3.69517707	-1.40330814	0.00000000
C	-3.69517707	1.40330816	0.00000000
C	-4.87542495	-0.70969378	0.00000000
C	-4.87542495	0.70969382	0.00000000
H	8.26608569	-1.25012563	0.00000000
H	8.26608565	1.25012569	0.00000000
H	6.12322356	-2.50212615	0.00000000
H	6.12322351	2.50212616	0.00000000
H	3.67209401	-2.50254092	0.00000000
H	3.67209403	2.50254089	0.00000000
H	1.21786108	-2.50362011	0.00000000
H	1.21786109	2.50362007	0.00000000
H	-1.23637179	-2.50254092	0.00000000
H	-1.23637179	2.50254090	0.00000000
H	-3.68750131	-2.50212615	0.00000000
H	-3.68750130	2.50212618	0.00000000
H	-5.83036345	-1.25012565	0.00000000
H	-5.83036344	1.25012567	0.00000000

5-acene (triplet), E = -839.0104609662

C	7.33746248	-0.70073359	0.00000000
C	7.33746248	0.70073359	0.00000000
C	6.13948944	-1.39605758	0.00000000
C	6.13948944	1.39605757	0.00000000
C	4.90790596	-0.71710729	0.00000000
C	4.90790597	0.71710728	0.00000000
C	3.67213820	-1.39703655	0.00000000
C	3.67213821	1.39703654	0.00000000
C	2.45081901	-0.72398235	0.00000000
C	2.45081902	0.72398236	0.00000000
C	1.21786124	-1.39901528	0.00000000
C	1.21786124	1.39901530	0.00000000
C	-0.01509677	-0.72398239	0.00000000
C	-0.01509677	0.72398240	0.00000000
C	-1.23641600	-1.39703661	0.00000000
C	-1.23641600	1.39703661	0.00000000
C	-2.47218374	-0.71710735	0.00000000
C	-2.47218375	0.71710736	0.00000000
C	-3.70376726	-1.39605776	0.00000000
C	-3.70376726	1.39605776	0.00000000
C	-4.90174031	-0.70073375	0.00000000
C	-4.90174032	0.70073374	0.00000000
H	8.28806419	-1.24842723	0.00000000
H	8.28806419	1.24842723	0.00000000
H	6.13189477	-2.49493576	0.00000000
H	6.13189477	2.49493575	0.00000000
H	3.67356978	-2.49726203	0.00000000
H	3.67356979	2.49726202	0.00000000
H	1.21786125	-2.49908913	0.00000000
H	1.21786125	2.49908915	0.00000000
H	-1.23784752	-2.49726209	0.00000000
H	-1.23784752	2.49726210	0.00000000
H	-3.69617263	-2.49493597	0.00000000
H	-3.69617264	2.49493597	0.00000000
H	-5.85234211	-1.24842740	0.00000000
H	-5.85234212	1.24842738	0.00000000

6-acene (singlet), E = -991.2816938455

C	7.31933057	-0.70921399	0.00000000
C	7.31933046	0.70921438	0.00000000
C	6.13800170	-1.40287706	0.00000000
C	6.13800148	1.40287727	0.00000000
C	4.89164682	-0.72295763	0.00000000
C	4.89164674	0.72295768	0.00000000
C	3.67785671	-1.40217524	0.00000000
C	3.67785656	1.40217509	0.00000000
C	2.44759589	-0.72627305	0.00000000
C	2.44759584	0.72627281	0.00000000
C	1.22529256	-1.40384887	0.00000000
C	1.22529251	1.40384853	0.00000000

C	-0.00000001	-0.72740813	0.00000000
C	-0.00000000	0.72740782	0.00000000
C	-1.22529257	-1.40384886	0.00000000
C	-1.22529252	1.40384854	0.00000000
C	-2.44759590	-0.72627304	0.00000000
C	-2.44759584	0.72627282	0.00000000
C	-3.67785671	-1.40217522	0.00000000
C	-3.67785657	1.40217510	0.00000000
C	-4.89164682	-0.72295761	0.00000000
C	-4.89164674	0.72295769	0.00000000
C	-6.13800168	-1.40287705	0.00000000
C	-6.13800148	1.40287727	0.00000000
C	-7.31933056	-0.70921400	0.00000000
C	-7.31933046	0.70921437	0.00000000
H	8.27409532	-1.24986004	0.00000000
H	8.27409515	1.24986056	0.00000000
H	6.13003265	-2.50170465	0.00000000
H	6.13003228	2.50170484	0.00000000
H	3.67874047	-2.50236185	0.00000000
H	3.67874019	2.50236169	0.00000000
H	1.22568039	-2.50388303	0.00000000
H	1.22568033	2.50388267	0.00000000
H	-1.22568041	-2.50388303	0.00000000
H	-1.22568033	2.50388268	0.00000000
H	-3.67874047	-2.50236183	0.00000000
H	-3.67874020	2.50236170	0.00000000
H	-6.13003262	-2.50170464	0.00000000
H	-6.13003228	2.50170485	0.00000000
H	-8.27409531	-1.24986006	0.00000000
H	-8.27409515	1.24986055	0.00000000

6-acene (triplet), E = -991.2601024865

C	7.33906748	-0.70324463	0.00000000
C	7.33906747	0.70324462	0.00000000
C	6.14642981	-1.39787415	0.00000000
C	6.14642981	1.39787417	0.00000000
C	4.91101817	-0.71822698	0.00000000
C	4.91101816	0.71822698	0.00000000
C	3.68054646	-1.39791931	0.00000000
C	3.68054646	1.39791931	0.00000000
C	2.46010370	-0.72386755	0.00000000
C	2.46010370	0.72386755	0.00000000
C	1.22562047	-1.39986582	0.00000000
C	1.22562047	1.39986581	0.00000000
C	-0.00000007	-0.72602238	0.00000000
C	-0.00000007	0.72602239	0.00000000
C	-1.22562034	-1.39986584	0.00000000
C	-1.22562034	1.39986584	0.00000000
C	-2.46010367	-0.72386759	0.00000000
C	-2.46010367	0.72386759	0.00000000
C	-3.68054646	-1.39791941	0.00000000
C	-3.68054646	1.39791941	0.00000000
C	-4.91101805	-0.71822708	0.00000000
C	-4.91101806	0.71822710	0.00000000
C	-6.14642989	-1.39787435	0.00000000
C	-6.14642990	1.39787436	0.00000000
C	-7.33906752	-0.70324478	0.00000000
C	-7.33906751	0.70324477	0.00000000
H	8.29097226	-1.24877040	0.00000000
H	8.29097226	1.24877039	0.00000000
H	6.13858400	-2.49674029	0.00000000
H	6.13858401	2.49674030	0.00000000
H	3.68163886	-2.49816873	0.00000000
H	3.68163887	2.49816873	0.00000000
H	1.22600709	-2.49997894	0.00000000
H	1.22600709	2.49997893	0.00000000
H	-1.22600688	-2.49997894	0.00000000
H	-1.22600689	2.49997895	0.00000000
H	-3.68163888	-2.49816884	0.00000000
H	-3.68163888	2.49816884	0.00000000
H	-6.13858414	-2.49674053	0.00000000
H	-6.13858417	2.49674054	0.00000000
H	-8.29097237	-1.24877057	0.00000000
H	-8.29097237	1.24877056	0.00000000

8-acene (singlet), E = -1295.7640364922

C	9.77260935	-0.70813249	0.00000000
C	9.77260944	0.70813206	0.00000000
C	8.58934436	-1.40191348	0.00000000
C	8.58934452	1.40191319	0.00000000
C	7.34532808	-0.72184489	0.00000000
C	7.34532816	0.72184473	0.00000000
C	6.12790040	-1.40116398	0.00000000

C	6.12790054	1.40116397	0.00000000
C	4.90109755	-0.72556090	0.00000000
C	4.90109761	0.72556100	0.00000000
C	3.67451333	-1.40284356	0.00000000
C	3.67451343	1.40284378	0.00000000
C	2.45182965	-0.72765555	0.00000000
C	2.45182968	0.72765583	0.00000000
C	1.22450804	-1.40324845	0.00000000
C	1.22450807	1.40324879	0.00000000
C	0.00000005	-0.72830371	0.00000000
C	0.00000006	0.72830404	0.00000000
C	-1.22450795	-1.40324845	0.00000000
C	-1.22450797	1.40324880	0.00000000
C	-2.45182957	-0.72765556	0.00000000
C	-2.45182960	0.72765584	0.00000000
C	-3.67451329	-1.40284356	0.00000000
C	-3.67451339	1.40284379	0.00000000
C	-4.90109754	-0.72556090	0.00000000
C	-4.90109760	0.72556101	0.00000000
C	-6.12790042	-1.40116400	0.00000000
C	-6.12790057	1.40116399	0.00000000
C	-7.34532813	-0.72184490	0.00000000
C	-7.34532821	0.72184474	0.00000000
C	-8.58934443	-1.40191349	0.00000000
C	-8.58934460	1.40191319	0.00000000
C	-9.77260945	-0.70813251	0.00000000
C	-9.77260953	0.70813205	0.00000000
H	10.72690391	-1.24957387	0.00000000
H	10.72690406	1.24957332	0.00000000
H	8.58129254	-2.50074445	0.00000000
H	8.58129284	2.50074416	0.00000000
H	6.12881821	-2.50137087	0.00000000
H	6.12881847	2.50137087	0.00000000
H	3.67515031	-2.50291630	0.00000000
H	3.67515051	2.50291653	0.00000000
H	1.22470470	-2.50331663	0.00000000
H	1.22470476	2.50331700	0.00000000
H	-1.22470463	-2.50331664	0.00000000
H	-1.22470468	2.50331701	0.00000000
H	-3.67515028	-2.50291630	0.00000000
H	-3.67515046	2.50291655	0.00000000
H	-6.12881822	-2.50137089	0.00000000
H	-6.12881849	2.50137090	0.00000000
H	-8.58129261	-2.50074446	0.00000000
H	-8.58129290	2.50074418	0.00000000
H	-10.72690400	-1.24957389	0.00000000
H	-10.72690414	1.24957333	0.00000000

8-acene (triplet), E = -1295.7515346798

C	9.78174855	-0.70606741	0.00000000
C	9.78174855	0.70606739	0.00000000
C	8.59475307	-1.40017757	0.00000000
C	8.59475306	1.40017755	0.00000000
C	7.35444274	-0.72010286	0.00000000
C	7.35444274	0.72010285	0.00000000
C	6.13127981	-1.39955100	0.00000000
C	6.13127981	1.39955099	0.00000000
C	4.90833302	-0.72433059	0.00000000
C	4.90833303	0.72433058	0.00000000
C	3.67649709	-1.40114363	0.00000000
C	3.67649710	1.40114364	0.00000000
C	2.45565207	-0.72647414	0.00000000
C	2.45565208	0.72647415	0.00000000
C	1.22521022	-1.40140908	0.00000000
C	1.22521022	1.40140911	0.00000000
C	0.00000021	-0.72701301	0.00000000
C	0.00000021	0.72701303	0.00000000
C	-1.22521007	-1.40140908	0.00000000
C	-1.22521007	1.40140910	0.00000000
C	-2.45565180	-0.72647415	0.00000000
C	-2.45565179	0.72647417	0.00000000
C	-3.67649696	-1.40114361	0.00000000
C	-3.67649697	1.40114364	0.00000000
C	-4.90833308	-0.72433058	0.00000000
C	-4.90833309	0.72433060	0.00000000
C	-6.13127982	-1.39955094	0.00000000
C	-6.13127984	1.39955096	0.00000000
C	-7.35444298	-0.72010279	0.00000000
C	-7.35444299	0.72010279	0.00000000
C	-8.59475318	-1.40017751	0.00000000
C	-8.59475321	1.40017750	0.00000000
C	-9.78174883	-0.70606736	0.00000000
C	-9.78174884	0.70606732	0.00000000
H	10.73502780	-1.24928857	0.00000000

H	10.73502780	1.24928855	0.00000000
H	8.58690810	-2.49901869	0.00000000
H	8.58690810	2.49901867	0.00000000
H	6.13222689	-2.49978233	0.00000000
H	6.13222690	2.49978231	0.00000000
H	3.67674907	-2.50125952	0.00000000
H	3.67674909	2.50125952	0.00000000
H	1.22514296	-2.50153020	0.00000000
H	1.22514297	2.50153022	0.00000000
H	-1.22514272	-2.50153021	0.00000000
H	-1.22514272	2.50153023	0.00000000
H	-3.67674893	-2.50125952	0.00000000
H	-3.67674895	2.50125954	0.00000000
H	-6.13222688	-2.49978227	0.00000000
H	-6.13222690	2.49978228	0.00000000
H	-8.58690823	-2.49901863	0.00000000
H	-8.58690828	2.49901861	0.00000000
H	-10.73502807	-1.24928855	0.00000000
H	-10.73502809	1.24928850	0.00000000

10-acene (singlet), E = -1600.2475455226

C	12.22378638	-0.70795687	0.00000000
C	12.22378719	0.70795388	0.00000000
C	11.04032854	-1.40179688	0.00000000
C	11.04033004	1.40179529	0.00000000
C	9.79671779	-0.72157235	0.00000000
C	9.79671844	0.72157179	0.00000000
C	8.57859931	-1.40092216	0.00000000
C	8.57860015	1.40092282	0.00000000
C	7.35291911	-0.72513585	0.00000000
C	7.35291928	0.72513676	0.00000000
C	6.12463410	-1.40240705	0.00000000
C	6.12463413	1.40240851	0.00000000
C	4.90423003	-0.72713187	0.00000000
C	4.90422979	0.72713314	0.00000000
C	3.67388584	-1.40258251	0.00000000
C	3.67388544	1.40258358	0.00000000
C	2.45270789	-0.72799667	0.00000000
C	2.45270761	0.72799766	0.00000000
C	1.22450132	-1.40246359	0.00000000
C	1.22450109	1.40246410	0.00000000
C	0.00000009	-0.72822430	0.00000000
C	0.00000007	0.72822508	0.00000000
C	-1.22450116	-1.40246359	0.00000000
C	-1.22450094	1.40246410	0.00000000
C	-2.45270773	-0.72799666	0.00000000
C	-2.45270745	0.72799767	0.00000000
C	-3.67388565	-1.40258250	0.00000000
C	-3.67388527	1.40258359	0.00000000
C	-4.90422983	-0.72713185	0.00000000
C	-4.90422960	0.72713315	0.00000000
C	-6.12463390	-1.40240705	0.00000000
C	-6.12463394	1.40240851	0.00000000
C	-7.35291891	-0.72513586	0.00000000
C	-7.35291909	0.72513675	0.00000000
C	-8.57859911	-1.40092217	0.00000000
C	-8.57859997	1.40092280	0.00000000
C	-9.79671760	-0.72157237	0.00000000
C	-9.79671825	0.72157177	0.00000000
C	-11.04032835	-1.40179691	0.00000000
C	-11.04032985	1.40179526	0.00000000
C	-12.22378619	-0.70795690	0.00000000
C	-12.22378700	0.70795384	0.00000000
H	13.17797516	-1.24962867	0.00000000
H	13.17797654	1.24962472	0.00000000
H	11.03243487	-2.50063110	0.00000000
H	11.03243738	2.50062967	0.00000000
H	8.57955195	-2.50113859	0.00000000
H	8.57955342	2.50113950	0.00000000
H	6.12508969	-2.50250544	0.00000000
H	6.12509003	2.50250709	0.00000000
H	3.67389764	-2.50269330	0.00000000
H	3.67389732	2.50269435	0.00000000
H	1.22445150	-2.50259005	0.00000000
H	1.22445127	2.50259034	0.00000000
H	-1.22445134	-2.50259005	0.00000000
H	-1.22445111	2.50259035	0.00000000
H	-3.67389745	-2.50269329	0.00000000
H	-3.67389715	2.50269435	0.00000000
H	-6.12508948	-2.50250543	0.00000000
H	-6.12508985	2.50250708	0.00000000
H	-8.57955174	-2.50113859	0.00000000
H	-8.57955324	2.50113948	0.00000000
H	-11.03243467	-2.50063112	0.00000000

H	-11.03243720	2.50062964	0.00000000
H	-13.17797497	-1.24962870	0.00000000
H	-13.17797635	1.24962469	0.00000000

10-acene (triplet), E = -1600.2381351729

C	12.22844482	-0.70714593	0.00000000
C	12.22844410	0.70714897	0.00000000
C	11.04349615	-1.40113939	0.00000000
C	11.04349477	1.40114121	0.00000000
C	9.80124219	-0.72099574	0.00000000
C	9.80124153	0.72099649	0.00000000
C	8.58113059	-1.40040528	0.00000000
C	8.58112956	1.40040493	0.00000000
C	7.35634244	-0.72485514	0.00000000
C	7.35634204	0.72485418	0.00000000
C	6.12693630	-1.40194473	0.00000000
C	6.12693580	1.40194302	0.00000000
C	4.90596383	-0.72675523	0.00000000
C	4.90596373	0.72675341	0.00000000
C	3.67578924	-1.40208554	0.00000000
C	3.67578926	1.40208342	0.00000000
C	2.45319069	-0.72719665	0.00000000
C	2.45319082	0.72719480	0.00000000
C	1.22527857	-1.40190967	0.00000000
C	1.22527897	1.40190799	0.00000000
C	0.00000029	-0.72718286	0.00000000
C	0.00000057	0.72718162	0.00000000
C	-1.22527861	-1.40190924	0.00000000
C	-1.22527806	1.40190842	0.00000000
C	-2.45319028	-0.72719593	0.00000000
C	-2.45318999	0.72719557	0.00000000
C	-3.67578919	-1.40208442	0.00000000
C	-3.67578872	1.40208452	0.00000000
C	-4.90596379	-0.72675415	0.00000000
C	-4.90596358	0.72675454	0.00000000
C	-6.12693611	-1.40194348	0.00000000
C	-6.12693586	1.40194425	0.00000000
C	-7.35634251	-0.72485421	0.00000000
C	-7.35634245	0.72485506	0.00000000
C	-8.58113019	-1.40040457	0.00000000
C	-8.58113019	1.40040557	0.00000000
C	-9.80124225	-0.72099561	0.00000000
C	-9.80124231	0.72099650	0.00000000
C	-11.04349575	-1.40113985	0.00000000
C	-11.04349590	1.40114066	0.00000000
C	-12.22844499	-0.70714706	0.00000000
C	-12.22844508	0.70714772	0.00000000
H	13.18221535	-1.24954413	0.00000000
H	13.18221408	1.24954809	0.00000000
H	11.03574635	-2.49997557	0.00000000
H	11.03574397	2.49997730	0.00000000
H	8.58219261	-2.50062419	0.00000000
H	8.58219086	2.50062367	0.00000000
H	6.12728033	-2.50204698	0.00000000
H	6.12727944	2.50204506	0.00000000
H	3.67556115	-2.50220080	0.00000000
H	3.67556113	2.50219850	0.00000000
H	1.22510803	-2.50204137	0.00000000
H	1.22510867	2.50203958	0.00000000
H	-1.22510833	-2.50204092	0.00000000
H	-1.22510742	2.50204009	0.00000000
H	-3.67556122	-2.50219961	0.00000000
H	-3.67556044	2.50219977	0.00000000
H	-6.12728004	-2.50204561	0.00000000
H	-6.12727957	2.50204647	0.00000000
H	-8.58219190	-2.50062338	0.00000000
H	-8.58219188	2.50062446	0.00000000
H	-11.03574542	-2.49997599	0.00000000
H	-11.03574568	2.49997684	0.00000000
H	-13.18221520	-1.24954585	0.00000000
H	-13.18221534	1.24954639	0.00000000

12-acene (singlet), E = -1904.7308013785

C	14.67386978	-0.70809290	0.00000000
C	14.67386851	0.70810065	0.00000000
C	13.49069852	-1.40192860	0.00000000
C	13.49069624	1.40193417	0.00000000
C	12.24679977	-0.72167960	0.00000000
C	12.24679888	0.72168352	0.00000000
C	11.02912088	-1.40103009	0.00000000
C	11.02911939	1.40103223	0.00000000
C	9.80315275	-0.72515155	0.00000000
C	9.80315215	0.72515247	0.00000000

C	8.57518404	-1.40248106	0.00000000
C	8.57518283	1.40248088	0.00000000
C	7.35486605	-0.72701206	0.00000000
C	7.35486543	0.72701071	0.00000000
C	6.12423917	-1.40256455	0.00000000
C	6.12423804	1.40256230	0.00000000
C	4.90402278	-0.72771528	0.00000000
C	4.90402222	0.72771203	0.00000000
C	3.67438449	-1.40224937	0.00000000
C	3.67438365	1.40224535	0.00000000
C	2.45215262	-0.72785536	0.00000000
C	2.45215229	0.72785070	0.00000000
C	1.22479026	-1.40198411	0.00000000
C	1.22478992	1.40197904	0.00000000
C	0.00000002	-0.72785024	0.00000000
C	0.00000000	0.72784501	0.00000000
C	-1.22479020	-1.40198416	0.00000000
C	-1.22478996	1.40197900	0.00000000
C	-2.45215258	-0.72785544	0.00000000
C	-2.45215230	0.72785061	0.00000000
C	-3.67438446	-1.40224949	0.00000000
C	-3.67438367	1.40224522	0.00000000
C	-4.90402277	-0.72771542	0.00000000
C	-4.90402223	0.72771189	0.00000000
C	-6.12423917	-1.40256471	0.00000000
C	-6.12423804	1.40256216	0.00000000
C	-7.35486606	-0.72701220	0.00000000
C	-7.35486542	0.72701056	0.00000000
C	-8.57518407	-1.40248119	0.00000000
C	-8.57518281	1.40248075	0.00000000
C	-9.80315278	-0.72515167	0.00000000
C	-9.80315213	0.72515236	0.00000000
C	-11.02912096	-1.40103017	0.00000000
C	-11.02911934	1.40103218	0.00000000
C	-12.24679982	-0.72167961	0.00000000
C	-12.24679885	0.72168351	0.00000000
C	-13.49069860	-1.40192855	0.00000000
C	-13.49069617	1.40193422	0.00000000
C	-14.67386983	-0.70809279	0.00000000
C	-14.67386848	0.70810075	0.00000000
H	15.62812940	-1.24964943	0.00000000
H	15.62812723	1.24965877	0.00000000
H	13.48284322	-2.50075916	0.00000000
H	13.48283922	2.50076454	0.00000000
H	11.03008851	-2.50124250	0.00000000
H	11.03008561	2.50124452	0.00000000
H	8.57560058	-2.50257735	0.00000000
H	8.57559833	2.50257717	0.00000000
H	6.12410427	-2.50267897	0.00000000
H	6.12410231	2.50267669	0.00000000
H	3.67409210	-2.50239148	0.00000000
H	3.67409064	2.50238733	0.00000000
H	1.22465338	-2.50214353	0.00000000
H	1.22465278	2.50213826	0.00000000
H	-1.22465327	-2.50214359	0.00000000
H	-1.22465286	2.50213822	0.00000000
H	-3.67409204	-2.50239160	0.00000000
H	-3.67409069	2.50238718	0.00000000
H	-6.12410427	-2.50267914	0.00000000
H	-6.12410231	2.50267654	0.00000000
H	-8.57560063	-2.50257750	0.00000000
H	-8.57559830	2.50257703	0.00000000
H	-11.03008863	-2.50124260	0.00000000
H	-11.03008551	2.50124444	0.00000000
H	-13.48284335	-2.50075914	0.00000000
H	-13.48283910	2.50076458	0.00000000
H	-15.62812948	-1.24964928	0.00000000
H	-15.62812716	1.24965893	0.00000000

12-acene (triplet), E = -1904.7231172373

C	14.67749723	-0.70750213	0.00000000
C	14.67749737	0.70749996	0.00000000
C	13.49320928	-1.40146060	0.00000000
C	13.49320966	1.40145868	0.00000000
C	12.25036181	-0.72127702	0.00000000
C	12.25036207	0.72127550	0.00000000
C	11.03118984	-1.40068919	0.00000000
C	11.03119038	1.40068802	0.00000000
C	9.80587809	-0.72504337	0.00000000
C	9.80587839	0.72504261	0.00000000
C	8.57723225	-1.40224104	0.00000000
C	8.57723292	1.40224068	0.00000000
C	7.35614355	-0.72696160	0.00000000
C	7.35614390	0.72696172	0.00000000

C	6.12636150	-1.40239161	0.00000000
C	6.12636239	1.40239211	0.00000000
C	4.90404852	-0.72739892	0.00000000
C	4.90404894	0.72739987	0.00000000
C	3.67612128	-1.40211394	0.00000000
C	3.67612225	1.40211529	0.00000000
C	2.45178541	-0.72717383	0.00000000
C	2.45178576	0.72717546	0.00000000
C	1.22547137	-1.40186509	0.00000000
C	1.22547223	1.40186697	0.00000000
C	-0.00000018	-0.72700526	0.00000000
C	0.00000007	0.72700727	0.00000000
C	-1.22547223	-1.40186498	0.00000000
C	-1.22547153	1.40186712	0.00000000
C	-2.45178578	-0.72717357	0.00000000
C	-2.45178560	0.72717573	0.00000000
C	-3.67612205	-1.40211353	0.00000000
C	-3.67612160	1.40211568	0.00000000
C	-4.90404881	-0.72739841	0.00000000
C	-4.90404876	0.72740035	0.00000000
C	-6.12636198	-1.40239097	0.00000000
C	-6.12636196	1.40239273	0.00000000
C	-7.35614362	-0.72696105	0.00000000
C	-7.35614379	0.72696228	0.00000000
C	-8.57723230	-1.40224050	0.00000000
C	-8.57723283	1.40224123	0.00000000
C	-9.80587799	-0.72504300	0.00000000
C	-9.80587839	0.72504297	0.00000000
C	-11.03118959	-1.40068901	0.00000000
C	-11.03119053	1.40068817	0.00000000
C	-12.25036160	-0.72127716	0.00000000
C	-12.25036215	0.72127536	0.00000000
C	-13.49320878	-1.40146104	0.00000000
C	-13.49321003	1.40145823	0.00000000
C	-14.67749689	-0.70750304	0.00000000
C	-14.67749756	0.70749906	0.00000000
H	15.63144081	-1.24959932	0.00000000
H	15.63144107	1.24959690	0.00000000
H	13.48545072	-2.50029284	0.00000000
H	13.48545137	2.50029085	0.00000000
H	11.03227353	-2.50090228	0.00000000
H	11.03227445	2.50090104	0.00000000
H	8.57767651	-2.50233530	0.00000000
H	8.57767769	2.50233487	0.00000000
H	6.12619900	-2.50249827	0.00000000
H	6.12620044	2.50249870	0.00000000
H	3.67581532	-2.50224241	0.00000000
H	3.67581683	2.50224376	0.00000000
H	1.22533656	-2.50200743	0.00000000
H	1.22533788	2.50200937	0.00000000
H	-1.22533782	-2.50200729	0.00000000
H	-1.22533676	2.50200951	0.00000000
H	-3.67581644	-2.50224193	0.00000000
H	-3.67581583	2.50224421	0.00000000
H	-6.12619969	-2.50249750	0.00000000
H	-6.12619980	2.50249943	0.00000000
H	-8.57767661	-2.50233463	0.00000000
H	-8.57767758	2.50233554	0.00000000
H	-11.03227311	-2.50090198	0.00000000
H	-11.03227477	2.50090130	0.00000000
H	-13.48544987	-2.50029319	0.00000000
H	-13.48545208	2.50029048	0.00000000
H	-15.63144027	-1.24960052	0.00000000
H	-15.63144146	1.24959569	0.00000000
14-acene (singlet), E = -2209.2138389610			
C	17.12416403	-0.70813977	0.00000000
C	17.12416349	0.70814100	0.00000000
C	15.94107369	-1.40199130	0.00000000
C	15.94107257	1.40199164	0.00000000
C	14.69709068	-0.72174107	0.00000000
C	14.69709003	0.72174037	0.00000000
C	13.47958120	-1.40110626	0.00000000
C	13.47958010	1.40110453	0.00000000
C	12.25343029	-0.72522031	0.00000000
C	12.25342978	0.72521795	0.00000000
C	11.02575150	-1.40258075	0.00000000
C	11.02575094	1.40257750	0.00000000
C	9.80515843	-0.72706651	0.00000000
C	9.80515831	0.72706331	0.00000000
C	8.57489721	-1.40268017	0.00000000
C	8.57489733	1.40267659	0.00000000
C	7.35443229	-0.72770463	0.00000000
C	7.35443254	0.72770167	0.00000000

C	6.12502831	-1.40234101	0.00000000
C	6.12502908	1.40233832	0.00000000
C	4.90289138	-0.72770897	0.00000000
C	4.90289192	0.72770738	0.00000000
C	3.67520083	-1.40196721	0.00000000
C	3.67520201	1.40196635	0.00000000
C	2.45135496	-0.72752532	0.00000000
C	2.45135566	0.72752572	0.00000000
C	1.22511210	-1.40175066	0.00000000
C	1.22511342	1.40175209	0.00000000
C	-0.00000033	-0.72743278	0.00000000
C	0.00000035	0.72743536	0.00000000
C	-1.22511329	-1.40174956	0.00000000
C	-1.22511218	1.40175319	0.00000000
C	-2.45135555	-0.72752330	0.00000000
C	-2.45135504	0.72752774	0.00000000
C	-3.67520173	-1.40196418	0.00000000
C	-3.67520109	1.40196940	0.00000000
C	-4.90289175	-0.72770547	0.00000000
C	-4.90289155	0.72771089	0.00000000
C	-6.12502867	-1.40233678	0.00000000
C	-6.12502872	1.40234254	0.00000000
C	-7.35443231	-0.72770052	0.00000000
C	-7.35443254	0.72770579	0.00000000
C	-8.57489682	-1.40267588	0.00000000
C	-8.57489772	1.40268088	0.00000000
C	-9.80515801	-0.72706301	0.00000000
C	-9.80515872	0.72706681	0.00000000
C	-11.02575035	-1.40257776	0.00000000
C	-11.02575209	1.40258048	0.00000000
C	-12.25342950	-0.72521874	0.00000000
C	-12.25343059	0.72521953	0.00000000
C	-13.47957942	-1.40110592	0.00000000
C	-13.47958189	1.40110486	0.00000000
C	-14.69708966	-0.72174252	0.00000000
C	-14.69709109	0.72173891	0.00000000
C	-15.94107160	-1.40199451	0.00000000
C	-15.94107469	1.40198843	0.00000000
C	-17.12416297	-0.70814481	0.00000000
C	-17.12416458	0.70813596	0.00000000
H	18.07843941	-1.24966972	0.00000000
H	18.07843843	1.24967168	0.00000000
H	15.93325014	-2.50081994	0.00000000
H	15.93324818	2.50082025	0.00000000
H	13.48058837	-2.50131522	0.00000000
H	13.48058666	2.50131336	0.00000000
H	11.02621024	-2.50267218	0.00000000
H	11.02620938	2.50266864	0.00000000
H	8.57477774	-2.50278849	0.00000000
H	8.57477795	2.50278461	0.00000000
H	6.12467827	-2.50247810	0.00000000
H	6.12467958	2.50247518	0.00000000
H	3.67489511	-2.50212754	0.00000000
H	3.67489708	2.50212653	0.00000000
H	1.22499673	-2.50192333	0.00000000
H	1.22499892	2.50192474	0.00000000
H	-1.22499873	-2.50192217	0.00000000
H	-1.22499689	2.50192593	0.00000000
H	-3.67489657	-2.50212433	0.00000000
H	-3.67489559	2.50212977	0.00000000
H	-6.12467884	-2.50247361	0.00000000
H	-6.12467900	2.50247967	0.00000000
H	-8.57477708	-2.50278389	0.00000000
H	-8.57477862	2.50278921	0.00000000
H	-11.02620828	-2.50266891	0.00000000
H	-11.02621134	2.50267191	0.00000000
H	-13.48058532	-2.50131470	0.00000000
H	-13.48058972	2.50131387	0.00000000
H	-15.93324648	-2.50082304	0.00000000
H	-15.93325186	2.50081714	0.00000000
H	-18.07843755	-1.24967616	0.00000000
H	-18.07844034	1.24966525	0.00000000
14-acene (triplet), E = -2209.2074898470			
C	17.12728720	-0.70765419	0.00000000
C	17.12728615	0.70767600	0.00000000
C	15.94331802	-1.40159292	0.00000000
C	15.94331502	1.40161260	0.00000000
C	14.70020707	-0.72137605	0.00000000
C	14.70020708	0.72139416	0.00000000
C	13.48143660	-1.40078583	0.00000000
C	13.48143317	1.40080173	0.00000000
C	12.25599124	-0.72507255	0.00000000
C	12.25599239	0.72508681	0.00000000

C	11.02752065	-1.40232477	0.00000000
C	11.02751688	1.40233770	0.00000000
C	9.80664430	-0.72701499	0.00000000
C	9.80664604	0.72702622	0.00000000
C	8.57673680	-1.40249096	0.00000000
C	8.57673317	1.40250171	0.00000000
C	7.35480186	-0.72755544	0.00000000
C	7.35480404	0.72756525	0.00000000
C	6.12676797	-1.40222850	0.00000000
C	6.12676489	1.40223780	0.00000000
C	4.90260011	-0.72736246	0.00000000
C	4.90260248	0.72737111	0.00000000
C	3.67646192	-1.40193224	0.00000000
C	3.67645876	1.40194041	0.00000000
C	2.45101305	-0.72701989	0.00000000
C	2.45101494	0.72702737	0.00000000
C	1.22557360	-1.40176921	0.00000000
C	1.22556941	1.40177577	0.00000000
C	-0.00000073	-0.72687240	0.00000000
C	0.00000096	0.72687847	0.00000000
C	-1.22556819	-1.40177029	0.00000000
C	-1.22557346	1.40177454	0.00000000
C	-2.45101476	-0.72702227	0.00000000
C	-2.45101272	0.72702544	0.00000000
C	-3.67645709	-1.40193525	0.00000000
C	-3.67646302	1.40193601	0.00000000
C	-4.90260218	-0.72736800	0.00000000
C	-4.90259991	0.72736672	0.00000000
C	-6.12676309	-1.40223422	0.00000000
C	-6.12676925	1.40223029	0.00000000
C	-7.35480366	-0.72756397	0.00000000
C	-7.35480179	0.72755741	0.00000000
C	-8.57673213	-1.40250122	0.00000000
C	-8.57673811	1.40249189	0.00000000
C	-9.80664557	-0.72702662	0.00000000
C	-9.80664470	0.72701423	0.00000000
C	-11.02751665	-1.40233975	0.00000000
C	-11.02752224	1.40232434	0.00000000
C	-12.25599170	-0.72508890	0.00000000
C	-12.25599194	0.72507003	0.00000000
C	-13.48143302	-1.40080513	0.00000000
C	-13.48143824	1.40078322	0.00000000
C	-14.70020664	-0.72139815	0.00000000
C	-14.70020810	0.72137232	0.00000000
C	-15.94331493	-1.40161773	0.00000000
C	-15.94331998	1.40158830	0.00000000
C	-17.12728619	-0.70768222	0.00000000
C	-17.12728839	0.70764873	0.00000000
H	18.08131551	-1.24960054	0.00000000
H	18.08131322	1.24962427	0.00000000
H	15.93554039	-2.50042227	0.00000000
H	15.93553719	2.50044195	0.00000000
H	13.48248970	-2.50099676	0.00000000
H	13.48248751	2.50101267	0.00000000
H	11.02796843	-2.50241707	0.00000000
H	11.02796785	2.50242999	0.00000000
H	8.57661349	-2.50259484	0.00000000
H	8.57661445	2.50260550	0.00000000
H	6.12649628	-2.50235362	0.00000000
H	6.12649694	2.50236290	0.00000000
H	3.67628354	-2.50207400	0.00000000
H	3.67628378	2.50208227	0.00000000
H	1.22552214	-2.50191951	0.00000000
H	1.22552216	2.50192617	0.00000000
H	-1.22551327	-2.50192072	0.00000000
H	-1.22551415	2.50192491	0.00000000
H	-3.67627817	-2.50207733	0.00000000
H	-3.67627993	2.50207801	0.00000000
H	-6.12649734	-2.50235965	0.00000000
H	-6.12649988	2.50235573	0.00000000
H	-8.57661800	-2.50260512	0.00000000
H	-8.57662157	2.50259587	0.00000000
H	-11.02796911	-2.50243194	0.00000000
H	-11.02797422	2.50241662	0.00000000
H	-13.48248514	-2.50101606	0.00000000
H	-13.48249157	2.50099424	0.00000000
H	-15.93553421	-2.50044715	0.00000000
H	-15.93554194	2.50041779	0.00000000
H	-18.08131365	-1.24962988	0.00000000
H	-18.08131780	1.24959315	0.00000000
16-acene (singlet), E = -2513.6968663768			
C	19.57470823	-0.70813190	0.00000000
C	19.57470970	0.70811637	0.00000000

C	18.39159076	-1.40199839	0.00000000
C	18.39159355	1.40198528	0.00000000
C	17.14765169	-0.72174025	0.00000000
C	17.14765301	0.72172945	0.00000000
C	15.93010717	-1.40111664	0.00000000
C	15.93010960	1.40110813	0.00000000
C	14.70397548	-0.72523256	0.00000000
C	14.70397664	0.72522620	0.00000000
C	13.47631362	-1.40259927	0.00000000
C	13.47631591	1.40259482	0.00000000
C	12.25565820	-0.72709219	0.00000000
C	12.25565937	0.72708989	0.00000000
C	11.02552510	-1.40271498	0.00000000
C	11.02552728	1.40271445	0.00000000
C	9.80487242	-0.72773749	0.00000000
C	9.80487350	0.72773896	0.00000000
C	8.57573864	-1.40240021	0.00000000
C	8.57574060	1.40240330	0.00000000
C	7.35329695	-0.72772523	0.00000000
C	7.35329792	0.72773019	0.00000000
C	6.12596663	-1.40204226	0.00000000
C	6.12596839	1.40204864	0.00000000
C	4.90183246	-0.72747291	0.00000000
C	4.90183337	0.72748095	0.00000000
C	3.67582164	-1.40179791	0.00000000
C	3.67582314	1.40180721	0.00000000
C	2.45076944	-0.72724115	0.00000000
C	2.45077016	0.72725163	0.00000000
C	1.22531970	-1.40168413	0.00000000
C	1.22532060	1.40169561	0.00000000
C	0.00000000	-0.72715244	0.00000000
C	0.00000026	0.72716434	0.00000000
C	-1.22531988	-1.40168366	0.00000000
C	-1.22531984	1.40169604	0.00000000
C	-2.45076931	-0.72724031	0.00000000
C	-2.45076952	0.72725242	0.00000000
C	-3.67582151	-1.40179661	0.00000000
C	-3.67582226	1.40180844	0.00000000
C	-4.90183200	-0.72747139	0.00000000
C	-4.90183256	0.72748240	0.00000000
C	-6.12596610	-1.40204041	0.00000000
C	-6.12596747	1.40205046	0.00000000
C	-7.35329626	-0.72772341	0.00000000
C	-7.35329710	0.72773203	0.00000000
C	-8.57573790	-1.40239819	0.00000000
C	-8.57573991	1.40240538	0.00000000
C	-9.80487177	-0.72773575	0.00000000
C	-9.80487298	0.72774080	0.00000000
C	-11.02552444	-1.40271328	0.00000000
C	-11.02552719	1.40271633	0.00000000
C	-12.25565787	-0.72709098	0.00000000
C	-12.25565947	0.72709126	0.00000000
C	-13.47631324	-1.40259836	0.00000000
C	-13.47631662	1.40259597	0.00000000
C	-14.70397558	-0.72523232	0.00000000
C	-14.70397744	0.72522661	0.00000000
C	-15.93010711	-1.40111696	0.00000000
C	-15.93011106	1.40110805	0.00000000
C	-17.14765216	-0.72174128	0.00000000
C	-17.14765436	0.72172857	0.00000000
C	-18.39159098	-1.40200016	0.00000000
C	-18.39159553	1.40198368	0.00000000
C	-19.57470900	-0.70813443	0.00000000
C	-19.57471135	0.70811392	0.00000000
H	20.52897344	-1.24967399	0.00000000
H	20.52897603	1.24965654	0.00000000
H	18.38377259	-2.50082504	0.00000000
H	18.38377754	2.50081203	0.00000000
H	15.93112049	-2.50132354	0.00000000
H	15.93112501	2.50131508	0.00000000
H	13.47678454	-2.50268809	0.00000000
H	13.47678872	2.50268364	0.00000000
H	11.02543140	-2.50281917	0.00000000
H	11.02543529	2.50281865	0.00000000
H	8.57542332	-2.50253110	0.00000000
H	8.57542681	2.50253426	0.00000000
H	6.12567574	-2.50219499	0.00000000
H	6.12567881	2.50220147	0.00000000
H	3.67565110	-2.50196418	0.00000000
H	3.67565356	2.50197369	0.00000000
H	1.22526715	-2.50185644	0.00000000
H	1.22526856	2.50186826	0.00000000
H	-1.22526758	-2.50185594	0.00000000

H	-1.22526749	2.50186869	0.00000000
H	-3.67565119	-2.50196280	0.00000000
H	-3.67565244	2.50197495	0.00000000
H	-6.12567534	-2.50219304	0.00000000
H	-6.12567782	2.50220338	0.00000000
H	-8.57542257	-2.50252902	0.00000000
H	-8.57542622	2.50253649	0.00000000
H	-11.02543056	-2.50281744	0.00000000
H	-11.02543543	2.50282075	0.00000000
H	-13.47678379	-2.50268719	0.00000000
H	-13.47678982	2.50268500	0.00000000
H	-15.93111991	-2.50132389	0.00000000
H	-15.93112695	2.50131518	0.00000000
H	-18.38377216	-2.50082685	0.00000000
H	-18.38378016	2.50081055	0.00000000
H	-20.52897394	-1.24967711	0.00000000
H	-20.52897804	1.24965356	0.00000000

16-acene (triplet), E = -2513.6914909572

C	19.57724124	-0.70777952	0.00000000
C	19.57724004	0.70779004	0.00000000
C	18.39350461	-1.40170487	0.00000000
C	18.39350137	1.40171313	0.00000000
C	17.15018895	-0.72146475	0.00000000
C	17.15018881	0.72147119	0.00000000
C	15.93172838	-1.40087069	0.00000000
C	15.93172462	1.40087464	0.00000000
C	14.70615237	-0.72510016	0.00000000
C	14.70615333	0.72510225	0.00000000
C	13.47783239	-1.40238938	0.00000000
C	13.47782803	1.40238998	0.00000000
C	12.25711105	-0.72702793	0.00000000
C	12.25711320	0.72702735	0.00000000
C	11.02704587	-1.40254512	0.00000000
C	11.02704115	1.40254444	0.00000000
C	9.80553214	-0.72762373	0.00000000
C	9.80553540	0.72762310	0.00000000
C	8.57717263	-1.40228446	0.00000000
C	8.57716785	1.40228444	0.00000000
C	7.35340234	-0.72751116	0.00000000
C	7.35340639	0.72751205	0.00000000
C	6.12711514	-1.40199656	0.00000000
C	6.12711002	1.40199884	0.00000000
C	4.90171955	-0.72719483	0.00000000
C	4.90172357	0.72719855	0.00000000
C	3.67653941	-1.40182698	0.00000000
C	3.67653323	1.40183240	0.00000000
C	2.45066777	-0.72695200	0.00000000
C	2.45067163	0.72695924	0.00000000
C	1.22556237	-1.40176410	0.00000000
C	1.22555503	1.40177248	0.00000000
C	-0.00000202	-0.72686725	0.00000000
C	0.00000198	0.72687680	0.00000000
C	-1.22555413	-1.40176388	0.00000000
C	-1.22556220	1.40177379	0.00000000
C	-2.45067200	-0.72695030	0.00000000
C	-2.45066795	0.72696027	0.00000000
C	-3.67653232	-1.40182587	0.00000000
C	-3.67654069	1.40183562	0.00000000
C	-4.90172438	-0.72719220	0.00000000
C	-4.90172084	0.72720109	0.00000000
C	-6.12711010	-1.40199365	0.00000000
C	-6.12711837	1.40200185	0.00000000
C	-7.35340754	-0.72750888	0.00000000
C	-7.35340511	0.72751546	0.00000000
C	-8.57716872	-1.40228092	0.00000000
C	-8.57717658	1.40228608	0.00000000
C	-9.80553626	-0.72762242	0.00000000
C	-9.80553535	0.72762509	0.00000000
C	-11.02704196	-1.40254436	0.00000000
C	-11.02704921	1.40254456	0.00000000
C	-12.25711281	-0.72702891	0.00000000
C	-12.25711348	0.72702553	0.00000000
C	-13.47782763	-1.40239336	0.00000000
C	-13.47783433	1.40238636	0.00000000
C	-14.70615099	-0.72510632	0.00000000
C	-14.70615293	0.72509481	0.00000000
C	-15.93172221	-1.40088052	0.00000000
C	-15.93172852	1.40086438	0.00000000
C	-17.15018529	-0.72147828	0.00000000
C	-17.15018785	0.72145713	0.00000000
C	-18.39349751	-1.40172197	0.00000000
C	-18.39350366	1.40169579	0.00000000
C	-19.57723606	-0.70780062	0.00000000

C	-19.57723899	0.70776943	0.00000000
H	20.53133197	-1.24961616	0.00000000
H	20.53132951	1.24962879	0.00000000
H	18.38571920	-2.50053184	0.00000000
H	18.38571566	2.50054013	0.00000000
H	15.93276527	-2.50107967	0.00000000
H	15.93276245	2.50108375	0.00000000
H	13.47827303	-2.50248060	0.00000000
H	13.47827213	2.50248129	0.00000000
H	11.02692050	-2.50264859	0.00000000
H	11.02692111	2.50264794	0.00000000
H	8.57690111	-2.50240913	0.00000000
H	8.57690174	2.50240921	0.00000000
H	6.12694726	-2.50213729	0.00000000
H	6.12694809	2.50213980	0.00000000
H	3.67649564	-2.50197641	0.00000000
H	3.67649665	2.50198208	0.00000000
H	1.22555915	-2.50191676	0.00000000
H	1.22555925	2.50192522	0.00000000
H	-1.22555977	-2.50191655	0.00000000
H	-1.22556091	2.50192644	0.00000000
H	-3.67649192	-2.50197544	0.00000000
H	-3.67649431	2.50198520	0.00000000
H	-6.12694211	-2.50213472	0.00000000
H	-6.12694572	2.50214299	0.00000000
H	-8.57690074	-2.50240585	0.00000000
H	-8.57690577	2.50241111	0.00000000
H	-11.02692359	-2.50264762	0.00000000
H	-11.02693031	2.50264788	0.00000000
H	-13.47827178	-2.50248410	0.00000000
H	-13.47828010	2.50247710	0.00000000
H	-15.93275694	-2.50108917	0.00000000
H	-15.93276667	2.50107300	0.00000000
H	-18.38570797	-2.50054870	0.00000000
H	-18.38571825	2.50052257	0.00000000
H	-20.53132576	-1.24963862	0.00000000
H	-20.53133103	1.24960331	0.00000000

18-acene (singlet), E = -2818.1799237367

C	22.02527054	-0.70810811	0.00000000
C	22.02526934	0.70811984	0.00000000
C	20.84214056	-1.40198407	0.00000000
C	20.84213823	1.40199375	0.00000000
C	19.59823288	-0.72171947	0.00000000
C	19.59823176	0.72172717	0.00000000
C	18.38065891	-1.40110702	0.00000000
C	18.38065680	1.40111277	0.00000000
C	17.15456269	-0.72521812	0.00000000
C	17.15456166	0.72522212	0.00000000
C	15.92687161	-1.40258962	0.00000000
C	15.92686978	1.40259183	0.00000000
C	14.70624110	-0.72708572	0.00000000
C	14.70624025	0.72708655	0.00000000
C	13.47609569	-1.40271142	0.00000000
C	13.47609428	1.40271073	0.00000000
C	12.25543824	-0.72774455	0.00000000
C	12.25543766	0.72774285	0.00000000
C	11.02633694	-1.40240890	0.00000000
C	11.02633594	1.40240614	0.00000000
C	9.80382272	-0.72774996	0.00000000
C	9.80382228	0.72774645	0.00000000
C	8.57661743	-1.40207362	0.00000000
C	8.57661671	1.40206940	0.00000000
C	7.35229968	-0.72751198	0.00000000
C	7.35229937	0.72750729	0.00000000
C	6.12654298	-1.40185837	0.00000000
C	6.12654259	1.40185316	0.00000000
C	4.90119607	-0.72726900	0.00000000
C	4.90119597	0.72726371	0.00000000
C	3.67608916	-1.40176116	0.00000000
C	3.67608908	1.40175555	0.00000000
C	2.45048827	-0.72711395	0.00000000
C	2.45048834	0.72710835	0.00000000
C	1.22538991	-1.40173172	0.00000000
C	1.22538997	1.40172611	0.00000000
C	-0.00000009	-0.72706286	0.00000000
C	-0.00000005	0.72705724	0.00000000
C	-1.22538999	-1.40173153	0.00000000
C	-1.22538992	1.40172603	0.00000000
C	-2.45048800	-0.72711369	0.00000000
C	-2.45048799	0.72710829	0.00000000
C	-3.67608840	-1.40176069	0.00000000
C	-3.67608820	1.40175542	0.00000000
C	-4.90119470	-0.72726858	0.00000000

C	-4.90119454	0.72726369	0.00000000
C	-6.12654104	-1.40185785	0.00000000
C	-6.12654058	1.40185312	0.00000000
C	-7.35229725	-0.72751160	0.00000000
C	-7.35229690	0.72750739	0.00000000
C	-8.57661473	-1.40207329	0.00000000
C	-8.57661400	1.40206959	0.00000000
C	-9.80381999	-0.72774978	0.00000000
C	-9.80381956	0.72774674	0.00000000
C	-11.02633450	-1.40240888	0.00000000
C	-11.02633353	1.40240663	0.00000000
C	-12.25543633	-0.72774458	0.00000000
C	-12.25543577	0.72774331	0.00000000
C	-13.47609452	-1.40271174	0.00000000
C	-13.47609322	1.40271140	0.00000000
C	-14.70624084	-0.72708598	0.00000000
C	-14.70624004	0.72708701	0.00000000
C	-15.92687226	-1.40259015	0.00000000
C	-15.92687058	1.40259246	0.00000000
C	-17.15456429	-0.72521853	0.00000000
C	-17.15456334	0.72522244	0.00000000
C	-18.38066126	-1.40110769	0.00000000
C	-18.38065931	1.40111324	0.00000000
C	-19.59823592	-0.72171995	0.00000000
C	-19.59823488	0.72172730	0.00000000
C	-20.84214413	-1.40198471	0.00000000
C	-20.84214199	1.40199390	0.00000000
C	-22.02527450	-0.70810858	0.00000000
C	-22.02527340	0.70811965	0.00000000
H	22.97953890	-1.24964292	0.00000000
H	22.97953681	1.24965619	0.00000000
H	20.83431363	-2.50080891	0.00000000
H	20.83430951	2.50081850	0.00000000
H	18.38166572	-2.50131166	0.00000000
H	18.38166197	2.50131732	0.00000000
H	15.92734039	-2.50267738	0.00000000
H	15.92733722	2.50267941	0.00000000
H	13.47600459	-2.50281433	0.00000000
H	13.47600201	2.50281344	0.00000000
H	11.02603667	-2.50253778	0.00000000
H	11.02603481	2.50253485	0.00000000
H	8.57635893	-2.50222288	0.00000000
H	8.57635771	2.50221851	0.00000000
H	6.12641375	-2.50201945	0.00000000
H	6.12641310	2.50201409	0.00000000
H	3.67605598	-2.50192734	0.00000000
H	3.67605566	2.50192163	0.00000000
H	1.22538858	-2.50189934	0.00000000
H	1.22538856	2.50189371	0.00000000
H	-1.22538847	-2.50189905	0.00000000
H	-1.22538824	2.50189353	0.00000000
H	-3.67605516	-2.50192665	0.00000000
H	-3.67605465	2.50192129	0.00000000
H	-6.12641194	-2.50201871	0.00000000
H	-6.12641121	2.50201387	0.00000000
H	-8.57635650	-2.50222254	0.00000000
H	-8.57635530	2.50221873	0.00000000
H	-11.02603452	-2.50253799	0.00000000
H	-11.02603272	2.50253561	0.00000000
H	-13.47600353	-2.50281508	0.00000000
H	-13.47600117	2.50281458	0.00000000
H	-15.92734095	-2.50267840	0.00000000
H	-15.92733805	2.50268056	0.00000000
H	-18.38166789	-2.50131276	0.00000000
H	-18.38166439	2.50131823	0.00000000
H	-20.83431712	-2.50080986	0.00000000
H	-20.83431332	2.50081897	0.00000000
H	-22.97954302	-1.24964363	0.00000000
H	-22.97954110	1.24965613	0.00000000
18-acene (triplet), E = -2818.1752330335			
C	22.02731440	-0.70788961	0.00000000
C	22.02731684	0.70785387	0.00000000
C	20.84374033	-1.40180351	0.00000000
C	20.84374524	1.40177178	0.00000000
C	19.60027903	-0.72154524	0.00000000
C	19.60028143	0.72151747	0.00000000
C	18.38204874	-1.40095087	0.00000000
C	18.38205340	1.40092703	0.00000000
C	17.15635053	-0.72513657	0.00000000
C	17.15635261	0.72511611	0.00000000
C	15.92818562	-1.40245144	0.00000000
C	15.92818974	1.40243449	0.00000000
C	14.70751073	-0.72704161	0.00000000

C	14.70751265	0.72702801	0.00000000
C	13.47740087	-1.40259249	0.00000000
C	13.47740467	1.40258235	0.00000000
C	12.25614639	-0.72765090	0.00000000
C	12.25614843	0.72764461	0.00000000
C	11.02755571	-1.40231654	0.00000000
C	11.02755927	1.40231421	0.00000000
C	9.80414887	-0.72757276	0.00000000
C	9.80415090	0.72757458	0.00000000
C	8.57759661	-1.40201953	0.00000000
C	8.57759962	1.40202572	0.00000000
C	7.35247480	-0.72729172	0.00000000
C	7.35247656	0.72730199	0.00000000
C	6.12719194	-1.40185281	0.00000000
C	6.12719419	1.40186746	0.00000000
C	4.90133771	-0.72706709	0.00000000
C	4.90133908	0.72708549	0.00000000
C	3.67642877	-1.40180189	0.00000000
C	3.67643017	1.40182417	0.00000000
C	2.45058386	-0.72695543	0.00000000
C	2.45058482	0.72698080	0.00000000
C	1.22549153	-1.40179993	0.00000000
C	1.22549198	1.40182854	0.00000000
C	0.00000018	-0.72692440	0.00000000
C	0.00000060	0.72695510	0.00000000
C	-1.22549063	-1.40179774	0.00000000
C	-1.22549145	1.40183085	0.00000000
C	-2.45058365	-0.72695127	0.00000000
C	-2.45058397	0.72698515	0.00000000
C	-3.67642801	-1.40179565	0.00000000
C	-3.67643035	1.40183079	0.00000000
C	-4.90133782	-0.72705919	0.00000000
C	-4.90133901	0.72709363	0.00000000
C	-6.12719142	-1.40184326	0.00000000
C	-6.12719539	1.40187739	0.00000000
C	-7.35247528	-0.72728106	0.00000000
C	-7.35247733	0.72731285	0.00000000
C	-8.57759617	-1.40200786	0.00000000
C	-8.57760179	1.40203761	0.00000000
C	-9.80414933	-0.72756104	0.00000000
C	-9.80415237	0.72758635	0.00000000
C	-11.02755478	-1.40230469	0.00000000
C	-11.02756218	1.40232597	0.00000000
C	-12.25614617	-0.72764048	0.00000000
C	-12.25615043	0.72765488	0.00000000
C	-13.47739877	-1.40258325	0.00000000
C	-13.47740813	1.40259127	0.00000000
C	-14.70750938	-0.72703526	0.00000000
C	-14.70751484	0.72703410	0.00000000
C	-15.92818231	-1.40244769	0.00000000
C	-15.92819324	1.40243777	0.00000000
C	-17.15634827	-0.72513640	0.00000000
C	-17.15635442	0.72511600	0.00000000
C	-18.38204471	-1.40095406	0.00000000
C	-18.38205645	1.40092336	0.00000000
C	-19.60027637	-0.72155198	0.00000000
C	-19.60028268	0.72151050	0.00000000
C	-20.84373579	-1.40181372	0.00000000
C	-20.84374797	1.40176124	0.00000000
C	-22.02731150	-0.70790318	0.00000000
C	-22.02731772	0.70784017	0.00000000
H	22.98145711	-1.24963888	0.00000000
H	22.98146137	1.24959995	0.00000000
H	20.83593380	-2.50062912	0.00000000
H	20.83594238	2.50059750	0.00000000
H	18.38307340	-2.50115753	0.00000000
H	18.38308160	2.50113384	0.00000000
H	15.92863363	-2.50254150	0.00000000
H	15.92864099	2.50252467	0.00000000
H	13.47728101	-2.50269586	0.00000000
H	13.47728786	2.50268577	0.00000000
H	11.02726830	-2.50244247	0.00000000
H	11.02727478	2.50244023	0.00000000
H	8.57740411	-2.50216197	0.00000000
H	8.57740982	2.50216836	0.00000000
H	6.12714886	-2.50200333	0.00000000
H	6.12715347	2.50201825	0.00000000
H	3.67646169	-2.50195456	0.00000000
H	3.67646475	2.50197717	0.00000000
H	1.22551395	-2.50195242	0.00000000
H	1.22551518	2.50198148	0.00000000
H	-1.22551345	-2.50195021	0.00000000
H	-1.22551445	2.50198393	0.00000000

H	-3.67646120	-2.50194825	0.00000000
H	-3.67646477	2.50198411	0.00000000
H	-6.12714823	-2.50199366	0.00000000
H	-6.12715470	2.50202856	0.00000000
H	-8.57740293	-2.50215007	0.00000000
H	-8.57741255	2.50218062	0.00000000
H	-11.02726594	-2.50243020	0.00000000
H	-11.02727890	2.50245233	0.00000000
H	-13.47727678	-2.50268611	0.00000000
H	-13.47729326	2.50269492	0.00000000
H	-15.92862776	-2.50253736	0.00000000
H	-15.92864702	2.50252798	0.00000000
H	-18.38306665	-2.50116051	0.00000000
H	-18.38308744	2.50113008	0.00000000
H	-20.83592631	-2.50063916	0.00000000
H	-20.83594806	2.50058689	0.00000000
H	-22.98145267	-1.24965501	0.00000000
H	-22.98146367	1.24958361	0.00000000

20-acene (singlet), E = -3122.6629883183

C	24.47578610	-0.70811182	0.00000000
C	24.47578576	0.70811572	0.00000000
C	23.29265965	-1.40199309	0.00000000
C	23.29265897	1.40199639	0.00000000
C	22.04875857	-0.72172047	0.00000000
C	22.04875826	0.72172312	0.00000000
C	20.83118480	-1.40111250	0.00000000
C	20.83118406	1.40111455	0.00000000
C	19.60509866	-0.72521666	0.00000000
C	19.60509821	0.72521797	0.00000000
C	18.37740232	-1.40259343	0.00000000
C	18.37740156	1.40259416	0.00000000
C	17.15679072	-0.72708141	0.00000000
C	17.15679030	0.72708172	0.00000000
C	15.92662946	-1.40271144	0.00000000
C	15.92662895	1.40271103	0.00000000
C	14.70599960	-0.72773925	0.00000000
C	14.70599948	0.72773874	0.00000000
C	13.47687469	-1.40240645	0.00000000
C	13.47687455	1.40240551	0.00000000
C	12.25439034	-0.72774934	0.00000000
C	12.25439039	0.72774833	0.00000000
C	11.02716661	-1.40207249	0.00000000
C	11.02716657	1.40207142	0.00000000
C	9.80285629	-0.72752188	0.00000000
C	9.80285625	0.72752071	0.00000000
C	8.57712297	-1.40186615	0.00000000
C	8.57712290	1.40186501	0.00000000
C	7.35171565	-0.72729532	0.00000000
C	7.35171557	0.72729418	0.00000000
C	6.12672637	-1.40178929	0.00000000
C	6.12672629	1.40178805	0.00000000
C	4.90095054	-0.72715242	0.00000000
C	4.90095051	0.72715128	0.00000000
C	3.67610304	-1.40178602	0.00000000
C	3.67610301	1.40178474	0.00000000
C	2.45042332	-0.72708791	0.00000000
C	2.45042335	0.72708668	0.00000000
C	1.22537663	-1.40180060	0.00000000
C	1.22537663	1.40179930	0.00000000
C	0.00000014	-0.72707136	0.00000000
C	0.00000014	0.72707006	0.00000000
C	-1.22537638	-1.40180065	0.00000000
C	-1.22537640	1.40179930	0.00000000
C	-2.45042314	-0.72708796	0.00000000
C	-2.45042317	0.72708667	0.00000000
C	-3.67610294	-1.40178610	0.00000000
C	-3.67610292	1.40178475	0.00000000
C	-4.90095056	-0.72715249	0.00000000
C	-4.90095053	0.72715128	0.00000000
C	-6.12672652	-1.40178936	0.00000000
C	-6.12672643	1.40178809	0.00000000
C	-7.35171592	-0.72729538	0.00000000
C	-7.35171583	0.72729421	0.00000000
C	-8.57712335	-1.40186619	0.00000000
C	-8.57712325	1.40186506	0.00000000
C	-9.80285673	-0.72752189	0.00000000
C	-9.80285670	0.72752075	0.00000000
C	-11.02716709	-1.40207249	0.00000000
C	-11.02716705	1.40207143	0.00000000
C	-12.25439081	-0.72774932	0.00000000
C	-12.25439085	0.72774832	0.00000000
C	-13.47687510	-1.40240639	0.00000000
C	-13.47687494	1.40240548	0.00000000

C	-14.70599991	-0.72773918	0.00000000
C	-14.70599980	0.72773874	0.00000000
C	-15.92662965	-1.40271133	0.00000000
C	-15.92662916	1.40271101	0.00000000
C	-17.15679078	-0.72708131	0.00000000
C	-17.15679036	0.72708171	0.00000000
C	-18.37740222	-1.40259332	0.00000000
C	-18.37740149	1.40259411	0.00000000
C	-19.60509844	-0.72521660	0.00000000
C	-19.60509800	0.72521794	0.00000000
C	-20.83118444	-1.40111244	0.00000000
C	-20.83118375	1.40111449	0.00000000
C	-22.04875812	-0.72172047	0.00000000
C	-22.04875783	0.72172303	0.00000000
C	-23.29265911	-1.40199309	0.00000000
C	-23.29265846	1.40199628	0.00000000
C	-24.47578550	-0.70811187	0.00000000
C	-24.47578518	0.70811563	0.00000000
H	25.43005520	-1.24964453	0.00000000
H	25.43005460	1.24964888	0.00000000
H	23.28483524	-2.50081694	0.00000000
H	23.28483395	2.50082023	0.00000000
H	20.83219181	-2.50131646	0.00000000
H	20.83219048	2.50131853	0.00000000
H	18.37786666	-2.50268082	0.00000000
H	18.37786566	2.50268148	0.00000000
H	15.92653366	-2.50281424	0.00000000
H	15.92653283	2.50281365	0.00000000
H	13.47656910	-2.50253496	0.00000000
H	13.47656859	2.50253388	0.00000000
H	11.02690904	-2.50222095	0.00000000
H	11.02690885	2.50221982	0.00000000
H	8.57700823	-2.50202560	0.00000000
H	8.57700823	2.50202443	0.00000000
H	6.12672533	-2.50195247	0.00000000
H	6.12672530	2.50195119	0.00000000
H	3.67614287	-2.50194913	0.00000000
H	3.67614276	2.50194780	0.00000000
H	1.22539728	-2.50196281	0.00000000
H	1.22539721	2.50196149	0.00000000
H	-1.22539703	-2.50196287	0.00000000
H	-1.22539702	2.50196150	0.00000000
H	-3.67614279	-2.50194925	0.00000000
H	-3.67614269	2.50194786	0.00000000
H	-6.12672549	-2.50195260	0.00000000
H	-6.12672541	2.50195127	0.00000000
H	-8.57700861	-2.50202568	0.00000000
H	-8.57700855	2.50202451	0.00000000
H	-11.02690949	-2.50222095	0.00000000
H	-11.02690931	2.50221983	0.00000000
H	-13.47656951	-2.50253488	0.00000000
H	-13.47656894	2.50253382	0.00000000
H	-15.92653384	-2.50281407	0.00000000
H	-15.92653302	2.50281358	0.00000000
H	-18.37786654	-2.50268065	0.00000000
H	-18.37786560	2.50268137	0.00000000
H	-20.83219144	-2.50131635	0.00000000
H	-20.83219021	2.50131842	0.00000000
H	-23.28483467	-2.50081690	0.00000000
H	-23.28483345	2.50082009	0.00000000
H	-25.43005462	-1.24964460	0.00000000
H	-25.43005404	1.24964877	0.00000000
20-acene (triplet), E = -3122.6588093357			
C	24.47752728	-0.70793792	0.00000000
C	24.47752893	0.70791075	0.00000000
C	23.29405368	-1.40185088	0.00000000
C	23.29405704	1.40182651	0.00000000
C	22.05050141	-0.72158425	0.00000000
C	22.05050302	0.72156248	0.00000000
C	20.83241802	-1.40099243	0.00000000
C	20.83242100	1.40097344	0.00000000
C	19.60663610	-0.72515637	0.00000000
C	19.60663711	0.72513910	0.00000000
C	18.37858276	-1.40249096	0.00000000
C	18.37858501	1.40247609	0.00000000
C	17.15791725	-0.72705230	0.00000000
C	17.15791798	0.72703919	0.00000000
C	15.92780953	-1.40262777	0.00000000
C	15.92781142	1.40261644	0.00000000
C	14.70668478	-0.72766970	0.00000000
C	14.70668598	0.72766077	0.00000000
C	13.47798756	-1.40234523	0.00000000
C	13.47798947	1.40233825	0.00000000

C	12.25478691	-0.72760786	0.00000000
C	12.25478860	0.72760365	0.00000000
C	11.02807919	-1.40203870	0.00000000
C	11.02808103	1.40203719	0.00000000
C	9.80316288	-0.72733847	0.00000000
C	9.80316474	0.72733984	0.00000000
C	8.57774954	-1.40186260	0.00000000
C	8.57775119	1.40186721	0.00000000
C	7.35203313	-0.72712345	0.00000000
C	7.35203498	0.72713111	0.00000000
C	6.12708042	-1.40181248	0.00000000
C	6.12708181	1.40182344	0.00000000
C	4.90125005	-0.72702583	0.00000000
C	4.90125192	0.72703978	0.00000000
C	3.67626264	-1.40182665	0.00000000
C	3.67626373	1.40184380	0.00000000
C	2.45061053	-0.72700538	0.00000000
C	2.45061228	0.72702526	0.00000000
C	1.22542025	-1.40184819	0.00000000
C	1.22542077	1.40187103	0.00000000
C	0.00000076	-0.72700523	0.00000000
C	0.00000220	0.72703012	0.00000000
C	-1.22541763	-1.40184614	0.00000000
C	-1.22541791	1.40187351	0.00000000
C	-2.45060973	-0.72700133	0.00000000
C	-2.45060882	0.72702988	0.00000000
C	-3.67626130	-1.40182069	0.00000000
C	-3.67626268	1.40185092	0.00000000
C	-4.90125106	-0.72701813	0.00000000
C	-4.90125087	0.72704838	0.00000000
C	-6.12708102	-1.40180324	0.00000000
C	-6.12708368	1.40183406	0.00000000
C	-7.35203622	-0.72711294	0.00000000
C	-7.35203684	0.72714247	0.00000000
C	-8.57775195	-1.40185104	0.00000000
C	-8.57775591	1.40187979	0.00000000
C	-9.80316741	-0.72732637	0.00000000
C	-9.80316889	0.72735237	0.00000000
C	-11.02808220	-1.40202621	0.00000000
C	-11.02808752	1.40204985	0.00000000
C	-12.25479123	-0.72759616	0.00000000
C	-12.25479369	0.72761516	0.00000000
C	-13.47798930	-1.40233383	0.00000000
C	-13.47799615	1.40234892	0.00000000
C	-14.70668684	-0.72766070	0.00000000
C	-14.70669060	0.72766904	0.00000000
C	-15.92780843	-1.40262005	0.00000000
C	-15.92781676	1.40262278	0.00000000
C	-17.15791592	-0.72704792	0.00000000
C	-17.15792086	0.72704254	0.00000000
C	-18.37857861	-1.40248915	0.00000000
C	-18.37858782	1.40247628	0.00000000
C	-19.60663197	-0.72515780	0.00000000
C	-19.60663718	0.72513662	0.00000000
C	-20.83241158	-1.40099709	0.00000000
C	-20.83242102	1.40096720	0.00000000
C	-22.05049554	-0.72159208	0.00000000
C	-22.05050050	0.72155378	0.00000000
C	-23.29404554	-1.40186165	0.00000000
C	-23.29405508	1.40181463	0.00000000
C	-24.47752011	-0.70795174	0.00000000
C	-24.47752497	0.70789650	0.00000000
H	25.43169762	-1.24963921	0.00000000
H	25.43170052	1.24960983	0.00000000
H	23.28624814	-2.50067533	0.00000000
H	23.28625380	2.50065108	0.00000000
H	20.83344360	-2.50119779	0.00000000
H	20.83344843	2.50117904	0.00000000
H	18.37903552	-2.50257986	0.00000000
H	18.37903994	2.50256517	0.00000000
H	15.92769443	-2.50273062	0.00000000
H	15.92769837	2.50271925	0.00000000
H	13.47769143	-2.50247122	0.00000000
H	13.47769521	2.50246413	0.00000000
H	11.02786475	-2.50218183	0.00000000
H	11.02786882	2.50218027	0.00000000
H	8.57768534	-2.50201420	0.00000000
H	8.57768970	2.50201881	0.00000000
H	6.12711206	-2.50196588	0.00000000
H	6.12711618	2.50197689	0.00000000
H	3.67631368	-2.50197885	0.00000000
H	3.67631728	2.50199615	0.00000000
H	1.22544168	-2.50199906	0.00000000

H	1.22544425	2.50202221	0.00000000
H	-1.22544112	-2.50199710	0.00000000
H	-1.22543995	2.50202495	0.00000000
H	-3.67631406	-2.50197309	0.00000000
H	-3.67631485	2.50200396	0.00000000
H	-6.12711379	-2.50195683	0.00000000
H	-6.12711687	2.50198837	0.00000000
H	-8.57768803	-2.50200263	0.00000000
H	-8.57769368	2.50203213	0.00000000
H	-11.02786684	-2.50216895	0.00000000
H	-11.02787553	2.50219338	0.00000000
H	-13.47769131	-2.50245901	0.00000000
H	-13.47770311	2.50247492	0.00000000
H	-15.92769126	-2.50272193	0.00000000
H	-15.92770546	2.50272530	0.00000000
H	-18.37902917	-2.50257729	0.00000000
H	-18.37904503	2.50256472	0.00000000
H	-20.83343437	-2.50120193	0.00000000
H	-20.83345152	2.50117211	0.00000000
H	-23.28623729	-2.50068566	0.00000000
H	-23.28625454	2.50063875	0.00000000
H	-25.43168895	-1.24965499	0.00000000
H	-25.43169752	1.24959324	0.00000000

22-acene (singlet), E = -3427.1460497984

C	26.92628394	-0.70811033	0.00000000
C	26.92628328	0.70811869	0.00000000
C	25.74316240	-1.40199758	0.00000000
C	25.74316111	1.40200486	0.00000000
C	24.49926488	-0.72171936	0.00000000
C	24.49926424	0.72172549	0.00000000
C	23.28169579	-1.40111619	0.00000000
C	23.28169449	1.40112123	0.00000000
C	22.05561179	-0.72521540	0.00000000
C	22.05561108	0.72521926	0.00000000
C	20.82792268	-1.40259766	0.00000000
C	20.82792136	1.40260040	0.00000000
C	19.60731323	-0.72707987	0.00000000
C	19.60731255	0.72708158	0.00000000
C	18.37715766	-1.40271658	0.00000000
C	18.37715656	1.40271720	0.00000000
C	17.15653587	-0.72773651	0.00000000
C	17.15653540	0.72773641	0.00000000
C	15.92740818	-1.40240987	0.00000000
C	15.92740748	1.40240892	0.00000000
C	14.70494063	-0.72774518	0.00000000
C	14.70494037	0.72774380	0.00000000
C	13.47770320	-1.40207379	0.00000000
C	13.47770281	1.40207193	0.00000000
C	12.25342081	-0.72751916	0.00000000
C	12.25342066	0.72751701	0.00000000
C	11.02766242	-1.40186623	0.00000000
C	11.02766216	1.40186383	0.00000000
C	9.80228645	-0.72729752	0.00000000
C	9.80228632	0.72729488	0.00000000
C	8.57727726	-1.40179125	0.00000000
C	8.57727700	1.40178839	0.00000000
C	7.35150964	-0.72716641	0.00000000
C	7.35150949	0.72716331	0.00000000
C	6.12668392	-1.40179834	0.00000000
C	6.12668362	1.40179499	0.00000000
C	4.90094427	-0.72711887	0.00000000
C	4.90094410	0.72711530	0.00000000
C	3.67601405	-1.40183330	0.00000000
C	3.67601377	1.40182945	0.00000000
C	2.45046259	-0.72711467	0.00000000
C	2.45046246	0.72711069	0.00000000
C	1.22533652	-1.40185955	0.00000000
C	1.22533641	1.40185536	0.00000000
C	0.00000006	-0.72711782	0.00000000
C	0.00000006	0.72711370	0.00000000
C	-1.22533643	-1.40185953	0.00000000
C	-1.22533630	1.40185538	0.00000000
C	-2.45046251	-0.72711463	0.00000000
C	-2.45046238	0.72711074	0.00000000
C	-3.67601400	-1.40183326	0.00000000
C	-3.67601371	1.40182952	0.00000000
C	-4.90094425	-0.72711883	0.00000000
C	-4.90094407	0.72711538	0.00000000
C	-6.12668394	-1.40179829	0.00000000
C	-6.12668363	1.40179509	0.00000000
C	-7.35150968	-0.72716636	0.00000000
C	-7.35150952	0.72716339	0.00000000
C	-8.57727732	-1.40179118	0.00000000

C	-8.57727706	1.40178849	0.00000000
C	-9.80228651	-0.72729746	0.00000000
C	-9.80228639	0.72729495	0.00000000
C	-11.02766249	-1.40186615	0.00000000
C	-11.02766224	1.40186390	0.00000000
C	-12.25342087	-0.72751910	0.00000000
C	-12.25342073	0.72751707	0.00000000
C	-13.47770324	-1.40207372	0.00000000
C	-13.47770288	1.40207197	0.00000000
C	-14.70494065	-0.72774511	0.00000000
C	-14.70494043	0.72774383	0.00000000
C	-15.92740819	-1.40240979	0.00000000
C	-15.92740752	1.40240895	0.00000000
C	-17.15653588	-0.72773646	0.00000000
C	-17.15653543	0.72773645	0.00000000
C	-18.37715764	-1.40271653	0.00000000
C	-18.37715658	1.40271722	0.00000000
C	-19.60731322	-0.72707985	0.00000000
C	-19.60731255	0.72708160	0.00000000
C	-20.82792264	-1.40259765	0.00000000
C	-20.82792137	1.40260040	0.00000000
C	-22.05561176	-0.72521542	0.00000000
C	-22.05561108	0.72521923	0.00000000
C	-23.28169574	-1.40111621	0.00000000
C	-23.28169450	1.40112116	0.00000000
C	-24.49926485	-0.72171942	0.00000000
C	-24.49926424	0.72172543	0.00000000
C	-25.74316234	-1.40199767	0.00000000
C	-25.74316114	1.40200476	0.00000000
C	-26.92628390	-0.70811046	0.00000000
C	-26.92628330	0.70811856	0.00000000
H	27.88055495	-1.24963959	0.00000000
H	27.88055379	1.24964885	0.00000000
H	25.73534135	-2.50082049	0.00000000
H	25.73533904	2.50082775	0.00000000
H	23.28270541	-2.50131942	0.00000000
H	23.28270309	2.50132446	0.00000000
H	20.82838730	-2.50268434	0.00000000
H	20.82838506	2.50268703	0.00000000
H	18.37705901	-2.50281868	0.00000000
H	18.37705713	2.50281913	0.00000000
H	15.92709955	-2.50253780	0.00000000
H	15.92709826	2.50253667	0.00000000
H	13.47744014	-2.50222170	0.00000000
H	13.47743937	2.50221970	0.00000000
H	11.02754301	-2.50202517	0.00000000
H	11.02754252	2.50202270	0.00000000
H	8.57727769	-2.50195375	0.00000000
H	8.57727722	2.50195088	0.00000000
H	6.12673894	-2.50196004	0.00000000
H	6.12673845	2.50195668	0.00000000
H	3.67606772	-2.50199287	0.00000000
H	3.67606727	2.50198896	0.00000000
H	1.22535753	-2.50201757	0.00000000
H	1.22535738	2.50201329	0.00000000
H	-1.22535747	-2.50201756	0.00000000
H	-1.22535724	2.50201332	0.00000000
H	-3.67606767	-2.50199284	0.00000000
H	-3.67606720	2.50198905	0.00000000
H	-6.12673897	-2.50196001	0.00000000
H	-6.12673845	2.50195679	0.00000000
H	-8.57727775	-2.50195370	0.00000000
H	-8.57727728	2.50195098	0.00000000
H	-11.02754307	-2.50202509	0.00000000
H	-11.02754260	2.50202278	0.00000000
H	-13.47744017	-2.50222162	0.00000000
H	-13.47743945	2.50221974	0.00000000
H	-15.92709956	-2.50253770	0.00000000
H	-15.92709828	2.50253669	0.00000000
H	-18.37705899	-2.50281861	0.00000000
H	-18.37705716	2.50281915	0.00000000
H	-20.82838724	-2.50268432	0.00000000
H	-20.82838509	2.50268701	0.00000000
H	-23.28270535	-2.50131943	0.00000000
H	-23.28270311	2.50132439	0.00000000
H	-25.73534126	-2.50082056	0.00000000
H	-25.73533910	2.50082764	0.00000000
H	-27.88055486	-1.24963974	0.00000000
H	-27.88055380	1.24964867	0.00000000
22-acene (triplet), E = -3427.1422800944			
C	26.92783024	-0.70795734	0.00000000
C	26.92783023	0.70796176	0.00000000
C	25.74442563	-1.40187276	0.00000000

C	25.74442559	1.40187712	0.00000000
C	24.50081416	-0.72159796	0.00000000
C	24.50081415	0.72160225	0.00000000
C	23.28282560	-1.40100882	0.00000000
C	23.28282554	1.40101310	0.00000000
C	22.05699114	-0.72515867	0.00000000
C	22.05699107	0.72516286	0.00000000
C	20.82900959	-1.40250689	0.00000000
C	20.82900940	1.40251097	0.00000000
C	19.60835261	-0.72705070	0.00000000
C	19.60835247	0.72705455	0.00000000
C	18.37824755	-1.40264347	0.00000000
C	18.37824722	1.40264711	0.00000000
C	17.15720745	-0.72767734	0.00000000
C	17.15720722	0.72768064	0.00000000
C	15.92844905	-1.40235828	0.00000000
C	15.92844857	1.40236121	0.00000000
C	14.70537413	-0.72762874	0.00000000
C	14.70537383	0.72763118	0.00000000
C	13.47858404	-1.40204926	0.00000000
C	13.47858340	1.40205117	0.00000000
C	12.25378092	-0.72736610	0.00000000
C	12.25378055	0.72736739	0.00000000
C	11.02830565	-1.40186875	0.00000000
C	11.02830491	1.40186940	0.00000000
C	9.80266861	-0.72715036	0.00000000
C	9.80266821	0.72715030	0.00000000
C	8.57768058	-1.40181424	0.00000000
C	8.57767978	1.40181346	0.00000000
C	7.35190388	-0.72705281	0.00000000
C	7.35190343	0.72705131	0.00000000
C	6.12690111	-1.40183022	0.00000000
C	6.12690029	1.40182797	0.00000000
C	4.90127591	-0.72704325	0.00000000
C	4.90127545	0.72704032	0.00000000
C	3.67611042	-1.40186482	0.00000000
C	3.67610961	1.40186109	0.00000000
C	2.45065002	-0.72706579	0.00000000
C	2.45064959	0.72706143	0.00000000
C	1.22535921	-1.40188829	0.00000000
C	1.22535848	1.40188320	0.00000000
C	-0.00000592	-0.72707855	0.00000000
C	-0.00000627	0.72707295	0.00000000
C	-1.22537069	-1.40188879	0.00000000
C	-1.22537127	1.40188255	0.00000000
C	-2.45066157	-0.72706677	0.00000000
C	-2.45066179	0.72706025	0.00000000
C	-3.67612138	-1.40186620	0.00000000
C	-3.67612175	1.40185924	0.00000000
C	-4.90128654	-0.72704512	0.00000000
C	-4.90128665	0.72703806	0.00000000
C	-6.12691081	-1.40183235	0.00000000
C	-6.12691091	1.40182502	0.00000000
C	-7.35191272	-0.72705532	0.00000000
C	-7.35191270	0.72704814	0.00000000
C	-8.57768804	-1.40181685	0.00000000
C	-8.57768783	1.40180962	0.00000000
C	-9.80267475	-0.72715327	0.00000000
C	-9.80267455	0.72714647	0.00000000
C	-11.02831006	-1.40187159	0.00000000
C	-11.02830948	1.40186502	0.00000000
C	-12.25378371	-0.72736909	0.00000000
C	-12.25378330	0.72736331	0.00000000
C	-13.47858512	-1.40205201	0.00000000
C	-13.47858414	1.40204680	0.00000000
C	-14.70537362	-0.72763149	0.00000000
C	-14.70537300	0.72762740	0.00000000
C	-15.92844723	-1.40236057	0.00000000
C	-15.92844578	1.40235746	0.00000000
C	-17.15720411	-0.72767931	0.00000000
C	-17.15720323	0.72767777	0.00000000
C	-18.37824328	-1.40264471	0.00000000
C	-18.37824137	1.40264453	0.00000000
C	-19.60834661	-0.72705130	0.00000000
C	-19.60834552	0.72705307	0.00000000
C	-20.82900271	-1.40250650	0.00000000
C	-20.82900044	1.40250998	0.00000000
C	-22.05698224	-0.72515744	0.00000000
C	-22.05698096	0.72516310	0.00000000
C	-23.28281597	-1.40100637	0.00000000
C	-23.28281339	1.40101410	0.00000000
C	-24.50080270	-0.72159463	0.00000000
C	-24.50080131	0.72160471	0.00000000

C	-25.74441383	-1.40186821	0.00000000
C	-25.74441109	1.40188069	0.00000000
C	-26.92781730	-0.70795198	0.00000000
C	-26.92781591	0.70796680	0.00000000
H	27.88202673	-1.24962228	0.00000000
H	27.88202671	1.24962673	0.00000000
H	25.73661770	-2.50069651	0.00000000
H	25.73661759	2.50070088	0.00000000
H	23.28385218	-2.50121360	0.00000000
H	23.28385206	2.50121792	0.00000000
H	20.82946590	-2.50259505	0.00000000
H	20.82946556	2.50259917	0.00000000
H	18.37813673	-2.50274546	0.00000000
H	18.37813616	2.50274915	0.00000000
H	15.92814874	-2.50248398	0.00000000
H	15.92814788	2.50248696	0.00000000
H	13.47835379	-2.50219265	0.00000000
H	13.47835264	2.50219461	0.00000000
H	11.02822623	-2.50202158	0.00000000
H	11.02822489	2.50202226	0.00000000
H	8.57770243	-2.50196948	0.00000000
H	8.57770098	2.50196869	0.00000000
H	6.12695338	-2.50198417	0.00000000
H	6.12695194	2.50198189	0.00000000
H	3.67615045	-2.50201657	0.00000000
H	3.67614903	2.50201279	0.00000000
H	1.22537330	-2.50203855	0.00000000
H	1.22537203	2.50203338	0.00000000
H	-1.22538427	-2.50203896	0.00000000
H	-1.22538525	2.50203261	0.00000000
H	-3.67616094	-2.50201768	0.00000000
H	-3.67616155	2.50201059	0.00000000
H	-6.12696269	-2.50198582	0.00000000
H	-6.12696282	2.50197833	0.00000000
H	-8.57770959	-2.50197142	0.00000000
H	-8.57770920	2.50196401	0.00000000
H	-11.02823051	-2.50202365	0.00000000
H	-11.02822946	2.50201689	0.00000000
H	-13.47835497	-2.50219465	0.00000000
H	-13.47835322	2.50218922	0.00000000
H	-15.92814730	-2.50248556	0.00000000
H	-15.92814471	2.50248224	0.00000000
H	-18.37813306	-2.50274601	0.00000000
H	-18.37812969	2.50274565	0.00000000
H	-20.82945980	-2.50259399	0.00000000
H	-20.82945583	2.50259733	0.00000000
H	-23.28384356	-2.50121056	0.00000000
H	-23.28383903	2.50121819	0.00000000
H	-25.73660690	-2.50069150	0.00000000
H	-25.73660204	2.50070391	0.00000000
H	-27.88201403	-1.24961583	0.00000000
H	-27.88201158	1.24963250	0.00000000

24-acene (singlet), E = -3731.6291088444

C	29.37679052	-0.70812044	0.00000000
C	29.37679151	0.70810458	0.00000000
C	28.19366881	-1.40201216	0.00000000
C	28.19367081	1.40199795	0.00000000
C	26.94977830	-0.72172838	0.00000000
C	26.94977936	0.72171604	0.00000000
C	25.73220735	-1.40112811	0.00000000
C	25.73220950	1.40111753	0.00000000
C	24.50612888	-0.72522218	0.00000000
C	24.50613004	0.72521355	0.00000000
C	23.27844189	-1.40260658	0.00000000
C	23.27844413	1.40259986	0.00000000
C	22.05783351	-0.72708317	0.00000000
C	22.05783468	0.72707827	0.00000000
C	20.82768526	-1.40272280	0.00000000
C	20.82768726	1.40271980	0.00000000
C	19.60706185	-0.72773666	0.00000000
C	19.60706277	0.72773513	0.00000000
C	18.37794281	-1.40241473	0.00000000
C	18.37794432	1.40241481	0.00000000
C	17.15547599	-0.72774217	0.00000000
C	17.15547663	0.72774335	0.00000000
C	15.92824317	-1.40207539	0.00000000
C	15.92824427	1.40207774	0.00000000
C	14.70396605	-0.72751277	0.00000000
C	14.70396653	0.72751601	0.00000000
C	13.47820462	-1.40186507	0.00000000
C	13.47820551	1.40186915	0.00000000
C	12.25284450	-0.72728891	0.00000000
C	12.25284493	0.72729376	0.00000000

C	11.02781942	-1.40178703	0.00000000
C	11.02782017	1.40179254	0.00000000
C	9.80208044	-0.72715707	0.00000000
C	9.80208081	0.72716319	0.00000000
C	8.57722763	-1.40179116	0.00000000
C	8.57722825	1.40179785	0.00000000
C	7.35152008	-0.72711384	0.00000000
C	7.35152037	0.72712098	0.00000000
C	6.12656749	-1.40182760	0.00000000
C	6.12656794	1.40183520	0.00000000
C	4.90102517	-0.72712087	0.00000000
C	4.90102537	0.72712878	0.00000000
C	3.67591868	-1.40186304	0.00000000
C	3.67591897	1.40187127	0.00000000
C	2.45052264	-0.72714062	0.00000000
C	2.45052276	0.72714901	0.00000000
C	1.22530140	-1.40188301	0.00000000
C	1.22530152	1.40189159	0.00000000
C	0.00000005	-0.72714973	0.00000000
C	0.00000007	0.72715833	0.00000000
C	-1.22530132	-1.40188298	0.00000000
C	-1.22530137	1.40189162	0.00000000
C	-2.45052255	-0.72714058	0.00000000
C	-2.45052262	0.72714906	0.00000000
C	-3.67591861	-1.40186297	0.00000000
C	-3.67591882	1.40187136	0.00000000
C	-4.90102509	-0.72712077	0.00000000
C	-4.90102525	0.72712889	0.00000000
C	-6.12656744	-1.40182745	0.00000000
C	-6.12656783	1.40183533	0.00000000
C	-7.35152002	-0.72711367	0.00000000
C	-7.35152029	0.72712114	0.00000000
C	-8.57722758	-1.40179097	0.00000000
C	-8.57722816	1.40179803	0.00000000
C	-9.80208037	-0.72715686	0.00000000
C	-9.80208073	0.72716338	0.00000000
C	-11.02781935	-1.40178679	0.00000000
C	-11.02782008	1.40179274	0.00000000
C	-12.25284442	-0.72728868	0.00000000
C	-12.25284484	0.72729398	0.00000000
C	-13.47820452	-1.40186483	0.00000000
C	-13.47820541	1.40186937	0.00000000
C	-14.70396593	-0.72751255	0.00000000
C	-14.70396642	0.72751623	0.00000000
C	-15.92824305	-1.40207519	0.00000000
C	-15.92824418	1.40207796	0.00000000
C	-17.15547589	-0.72774198	0.00000000
C	-17.15547654	0.72774355	0.00000000
C	-18.37794270	-1.40241457	0.00000000
C	-18.37794427	1.40241501	0.00000000
C	-19.60706179	-0.72773654	0.00000000
C	-19.60706275	0.72773528	0.00000000
C	-20.82768521	-1.40272273	0.00000000
C	-20.82768732	1.40271992	0.00000000
C	-22.05783354	-0.72708315	0.00000000
C	-22.05783477	0.72707833	0.00000000
C	-23.27844192	-1.40260664	0.00000000
C	-23.27844431	1.40259986	0.00000000
C	-24.50612899	-0.72522229	0.00000000
C	-24.50613025	0.72521348	0.00000000
C	-25.73220747	-1.40112830	0.00000000
C	-25.73220977	1.40111742	0.00000000
C	-26.94977849	-0.72172860	0.00000000
C	-26.94977963	0.72171585	0.00000000
C	-28.19366899	-1.40201245	0.00000000
C	-28.19367114	1.40199771	0.00000000
C	-29.37679076	-0.70812080	0.00000000
C	-29.37679183	0.70810424	0.00000000
H	30.33105972	-1.24965159	0.00000000
H	30.33106150	1.24963436	0.00000000
H	28.18585192	-2.50083437	0.00000000
H	28.18585552	2.50082015	0.00000000
H	25.73321953	-2.50133070	0.00000000
H	25.73322335	2.50132009	0.00000000
H	23.27890685	-2.50269263	0.00000000
H	23.27891072	2.50268596	0.00000000
H	20.82758510	-2.50282402	0.00000000
H	20.82758858	2.50282121	0.00000000
H	18.37763113	-2.50254167	0.00000000
H	18.37763388	2.50254198	0.00000000
H	15.92797753	-2.50222244	0.00000000
H	15.92797960	2.50222497	0.00000000
H	13.47807927	-2.50202318	0.00000000

H	13.47808089	2.50202737	0.00000000
H	11.02781357	-2.50194879	0.00000000
H	11.02781489	2.50195438	0.00000000
H	8.57727826	-2.50195224	0.00000000
H	8.57727932	2.50195900	0.00000000
H	6.12662410	-2.50198629	0.00000000
H	6.12662487	2.50199396	0.00000000
H	3.67595663	-2.50201949	0.00000000
H	3.67595712	2.50202779	0.00000000
H	1.22531421	-2.50203819	0.00000000
H	1.22531442	2.50204683	0.00000000
H	-1.22531416	-2.50203816	0.00000000
H	-1.22531426	2.50204686	0.00000000
H	-3.67595659	-2.50201943	0.00000000
H	-3.67595696	2.50202789	0.00000000
H	-6.12662407	-2.50198614	0.00000000
H	-6.12662474	2.50199409	0.00000000
H	-8.57727821	-2.50195204	0.00000000
H	-8.57727921	2.50195918	0.00000000
H	-11.02781350	-2.50194855	0.00000000
H	-11.02781477	2.50195459	0.00000000
H	-13.47807916	-2.50202294	0.00000000
H	-13.47808079	2.50202760	0.00000000
H	-15.92797741	-2.50222224	0.00000000
H	-15.92797953	2.50222520	0.00000000
H	-18.37763101	-2.50254152	0.00000000
H	-18.37763387	2.50254221	0.00000000
H	-20.82758502	-2.50282397	0.00000000
H	-20.82758869	2.50282136	0.00000000
H	-23.27890684	-2.50269271	0.00000000
H	-23.27891095	2.50268601	0.00000000
H	-25.73321960	-2.50133091	0.00000000
H	-25.73322366	2.50132001	0.00000000
H	-28.18585204	-2.50083469	0.00000000
H	-28.18585591	2.50081992	0.00000000
H	-30.33105995	-1.24965202	0.00000000
H	-30.33106186	1.24963398	0.00000000

24-acene (triplet), E = -3731.6256769264

C	29.37816990	-0.70798165	0.00000000
C	29.37817001	0.70798295	0.00000000
C	28.19481149	-1.40189706	0.00000000
C	28.19481165	1.40189870	0.00000000
C	26.95116096	-0.72161897	0.00000000
C	26.95116105	0.72162091	0.00000000
C	25.73324175	-1.40103167	0.00000000
C	25.73324177	1.40103409	0.00000000
C	24.50737295	-0.72516850	0.00000000
C	24.50737299	0.72517123	0.00000000
C	23.27944255	-1.40252585	0.00000000
C	23.27944256	1.40252916	0.00000000
C	22.05879769	-0.72705513	0.00000000
C	22.05879772	0.72705870	0.00000000
C	20.82868999	-1.40265930	0.00000000
C	20.82869004	1.40266310	0.00000000
C	19.60772145	-0.72768648	0.00000000
C	19.60772152	0.72769026	0.00000000
C	18.37890874	-1.40237234	0.00000000
C	18.37890886	1.40237590	0.00000000
C	17.15593162	-0.72764763	0.00000000
C	17.15593176	0.72765084	0.00000000
C	15.92907990	-1.40205787	0.00000000
C	15.92908009	1.40206060	0.00000000
C	14.70435672	-0.72739070	0.00000000
C	14.70435693	0.72739282	0.00000000
C	13.47884844	-1.40187286	0.00000000
C	13.47884870	1.40187440	0.00000000
C	12.25325222	-0.72717144	0.00000000
C	12.25325247	0.72717225	0.00000000
C	11.02826769	-1.40181397	0.00000000
C	11.02826801	1.40181419	0.00000000
C	9.80250402	-0.72706485	0.00000000
C	9.80250428	0.72706435	0.00000000
C	8.57751923	-1.40182547	0.00000000
C	8.57751961	1.40182444	0.00000000
C	7.35190803	-0.72704835	0.00000000
C	7.35190827	0.72704665	0.00000000
C	6.12674770	-1.40185818	0.00000000
C	6.12674816	1.40185599	0.00000000
C	4.90131882	-0.72707285	0.00000000
C	4.90131905	0.72707016	0.00000000
C	3.67601834	-1.40188485	0.00000000
C	3.67601885	1.40188163	0.00000000
C	2.45068017	-0.72710036	0.00000000

C	2.45068044	0.72709680	0.00000000
C	1.22533435	-1.40189833	0.00000000
C	1.22533498	1.40189423	0.00000000
C	0.00000139	-0.72711159	0.00000000
C	0.00000174	0.72710735	0.00000000
C	-1.22533201	-1.40189873	0.00000000
C	-1.22533120	1.40189401	0.00000000
C	-2.45067782	-0.72710102	0.00000000
C	-2.45067736	0.72709640	0.00000000
C	-3.67601684	-1.40188596	0.00000000
C	-3.67601578	1.40188099	0.00000000
C	-4.90131752	-0.72707399	0.00000000
C	-4.90131689	0.72706937	0.00000000
C	-6.12674741	-1.40185976	0.00000000
C	-6.12674611	1.40185491	0.00000000
C	-7.35190783	-0.72704977	0.00000000
C	-7.35190706	0.72704551	0.00000000
C	-8.57751982	-1.40182724	0.00000000
C	-8.57751835	1.40182294	0.00000000
C	-9.80250442	-0.72706646	0.00000000
C	-9.80250352	0.72706282	0.00000000
C	-11.02826847	-1.40181585	0.00000000
C	-11.02826694	1.40181230	0.00000000
C	-12.25325250	-0.72717326	0.00000000
C	-12.25325156	0.72717034	0.00000000
C	-13.47884880	-1.40187488	0.00000000
C	-13.47884730	1.40187220	0.00000000
C	-14.70435650	-0.72739277	0.00000000
C	-14.70435560	0.72739062	0.00000000
C	-15.92907972	-1.40206008	0.00000000
C	-15.92907833	1.40205835	0.00000000
C	-17.15593110	-0.72764985	0.00000000
C	-17.15593030	0.72764867	0.00000000
C	-18.37890850	-1.40237448	0.00000000
C	-18.37890731	1.40237399	0.00000000
C	-19.60772128	-0.72768843	0.00000000
C	-19.60772065	0.72768859	0.00000000
C	-20.82869044	-1.40266092	0.00000000
C	-20.82868948	1.40266204	0.00000000
C	-22.05879853	-0.72705613	0.00000000
C	-22.05879807	0.72705814	0.00000000
C	-23.27944420	-1.40252633	0.00000000
C	-23.27944347	1.40252940	0.00000000
C	-24.50737513	-0.72516804	0.00000000
C	-24.50737476	0.72517217	0.00000000
C	-25.73324466	-1.40103072	0.00000000
C	-25.73324405	1.40103578	0.00000000
C	-26.95116427	-0.72161716	0.00000000
C	-26.95116393	0.72162316	0.00000000
C	-28.19481546	-1.40189477	0.00000000
C	-28.19481479	1.40190157	0.00000000
C	-29.37817393	-0.70797865	0.00000000
C	-29.37817358	0.70798621	0.00000000
H	30.33237199	-1.24962576	0.00000000
H	30.33237219	1.24962695	0.00000000
H	28.18700789	-2.50071909	0.00000000
H	28.18700813	2.50072074	0.00000000
H	25.73426757	-2.50123465	0.00000000
H	25.73426762	2.50123707	0.00000000
H	23.27990130	-2.50261235	0.00000000
H	23.27990155	2.50261564	0.00000000
H	20.82858008	-2.50275997	0.00000000
H	20.82858035	2.50276372	0.00000000
H	18.37860864	-2.50249696	0.00000000
H	18.37860890	2.50250047	0.00000000
H	15.92884950	-2.50220067	0.00000000
H	15.92884985	2.50220336	0.00000000
H	13.47876126	-2.50202501	0.00000000
H	13.47876173	2.50202651	0.00000000
H	11.02828099	-2.50196862	0.00000000
H	11.02828163	2.50196881	0.00000000
H	8.57756435	-2.50197908	0.00000000
H	8.57756515	2.50197801	0.00000000
H	6.12678361	-2.50200967	0.00000000
H	6.12678463	2.50200743	0.00000000
H	3.67603554	-2.50203468	0.00000000
H	3.67603664	2.50203137	0.00000000
H	1.22533854	-2.50204735	0.00000000
H	1.22533978	2.50204312	0.00000000
H	-1.22533690	-2.50204785	0.00000000
H	-1.22533535	2.50204296	0.00000000
H	-3.67603482	-2.50203602	0.00000000
H	-3.67603282	2.50203086	0.00000000

H	-6.12678414	-2.50201151	0.00000000
H	-6.12678175	2.50200647	0.00000000
H	-8.57756571	-2.50198104	0.00000000
H	-8.57756311	2.50197657	0.00000000
H	-11.02828249	-2.50197056	0.00000000
H	-11.02827984	2.50196691	0.00000000
H	-13.47876225	-2.50202700	0.00000000
H	-13.47875969	2.50202429	0.00000000
H	-15.92884990	-2.50220286	0.00000000
H	-15.92884752	2.50220117	0.00000000
H	-18.37860894	-2.50249919	0.00000000
H	-18.37860682	2.50249877	0.00000000
H	-20.82858111	-2.50276179	0.00000000
H	-20.82857922	2.50276299	0.00000000
H	-23.27990348	-2.50261309	0.00000000
H	-23.27990193	2.50261622	0.00000000
H	-25.73427077	-2.50123396	0.00000000
H	-25.73426960	2.50123906	0.00000000
H	-28.18701220	-2.50071702	0.00000000
H	-28.18701100	2.50072381	0.00000000
H	-30.33237636	-1.24962252	0.00000000
H	-30.33237571	1.24963056	0.00000000

26-acene (singlet), E = -4036.1121678692

C	31.82728718	-0.70812585	0.00000000
C	31.82728857	0.70810222	0.00000000
C	30.64416413	-1.40202083	0.00000000
C	30.64416695	1.40199953	0.00000000
C	29.40027876	-0.72173048	0.00000000
C	29.40028026	0.72171177	0.00000000
C	28.18270985	-1.40113381	0.00000000
C	28.18271286	1.40111761	0.00000000
C	26.95663389	-0.72522325	0.00000000
C	26.95663550	0.72520972	0.00000000
C	25.72895262	-1.40261116	0.00000000
C	25.72895566	1.40260027	0.00000000
C	24.50834216	-0.72708276	0.00000000
C	24.50834372	0.72707440	0.00000000
C	23.27820340	-1.40272623	0.00000000
C	23.27820618	1.40272046	0.00000000
C	22.05757592	-0.72773501	0.00000000
C	22.05757726	0.72773140	0.00000000
C	20.82846739	-1.40241825	0.00000000
C	20.82846966	1.40241691	0.00000000
C	19.60599784	-0.72774016	0.00000000
C	19.60599886	0.72774054	0.00000000
C	18.37877239	-1.40207924	0.00000000
C	18.37877417	1.40208145	0.00000000
C	17.15449738	-0.72750956	0.00000000
C	17.15449817	0.72751318	0.00000000
C	15.92873920	-1.40186679	0.00000000
C	15.92874060	1.40187177	0.00000000
C	14.70338306	-0.72728442	0.00000000
C	14.70338369	0.72729058	0.00000000
C	13.47836154	-1.40178794	0.00000000
C	13.47836270	1.40179518	0.00000000
C	12.25263022	-0.72715292	0.00000000
C	12.25263076	0.72716112	0.00000000
C	11.02777130	-1.40179158	0.00000000
C	11.02777222	1.40180066	0.00000000
C	9.80208099	-0.72710751	0.00000000
C	9.80208140	0.72711730	0.00000000
C	8.57711179	-1.40182521	0.00000000
C	8.57711244	1.40183570	0.00000000
C	7.35159719	-0.72711437	0.00000000
C	7.35159746	0.72712531	0.00000000
C	6.12646449	-1.40185938	0.00000000
C	6.12646488	1.40187079	0.00000000
C	4.90109891	-0.72713870	0.00000000
C	4.90109905	0.72715036	0.00000000
C	3.67585645	-1.40188115	0.00000000
C	3.67585662	1.40189305	0.00000000
C	2.45056256	-0.72715928	0.00000000
C	2.45056263	0.72717124	0.00000000
C	1.22528142	-1.40189092	0.00000000
C	1.22528147	1.40190297	0.00000000
C	0.00000004	-0.72716694	0.00000000
C	0.00000004	0.72717898	0.00000000
C	-1.22528135	-1.40189092	0.00000000
C	-1.22528142	1.40190296	0.00000000
C	-2.45056251	-0.72715930	0.00000000
C	-2.45056256	0.72717122	0.00000000
C	-3.67585638	-1.40188121	0.00000000
C	-3.67585657	1.40189301	0.00000000

C	-4.90109884	-0.72713876	0.00000000
C	-4.90109898	0.72715030	0.00000000
C	-6.12646440	-1.40185947	0.00000000
C	-6.12646479	1.40187074	0.00000000
C	-7.35159710	-0.72711443	0.00000000
C	-7.35159737	0.72712526	0.00000000
C	-8.57711169	-1.40182529	0.00000000
C	-8.57711235	1.40183564	0.00000000
C	-9.80208090	-0.72710758	0.00000000
C	-9.80208132	0.72711723	0.00000000
C	-11.02777123	-1.40179165	0.00000000
C	-11.02777214	1.40180061	0.00000000
C	-12.25263018	-0.72715298	0.00000000
C	-12.25263072	0.72716107	0.00000000
C	-13.47836152	-1.40178800	0.00000000
C	-13.47836268	1.40179513	0.00000000
C	-14.70338306	-0.72728448	0.00000000
C	-14.70338370	0.72729053	0.00000000
C	-15.92873923	-1.40186685	0.00000000
C	-15.92874064	1.40187172	0.00000000
C	-17.15449744	-0.72750964	0.00000000
C	-17.15449823	0.72751310	0.00000000
C	-18.37877248	-1.40207932	0.00000000
C	-18.37877424	1.40208137	0.00000000
C	-19.60599793	-0.72774024	0.00000000
C	-19.60599896	0.72774047	0.00000000
C	-20.82846751	-1.40241831	0.00000000
C	-20.82846975	1.40241685	0.00000000
C	-22.05757603	-0.72773505	0.00000000
C	-22.05757735	0.72773135	0.00000000
C	-23.27820351	-1.40272623	0.00000000
C	-23.27820626	1.40272044	0.00000000
C	-24.50834224	-0.72708274	0.00000000
C	-24.50834380	0.72707441	0.00000000
C	-25.72895269	-1.40261111	0.00000000
C	-25.72895571	1.40260030	0.00000000
C	-26.95663394	-0.72522320	0.00000000
C	-26.95663553	0.72520975	0.00000000
C	-28.18270987	-1.40113375	0.00000000
C	-28.18271287	1.40111765	0.00000000
C	-29.40027876	-0.72173042	0.00000000
C	-29.40028028	0.72171183	0.00000000
C	-30.64416413	-1.40202077	0.00000000
C	-30.64416695	1.40199958	0.00000000
C	-31.82728717	-0.70812579	0.00000000
C	-31.82728856	0.70810227	0.00000000
H	32.78156133	-1.24964783	0.00000000
H	32.78156382	1.24962228	0.00000000
H	30.63633610	-2.50084104	0.00000000
H	30.63634115	2.50081971	0.00000000
H	28.18371369	-2.50133457	0.00000000
H	28.18371902	2.50131836	0.00000000
H	25.72941243	-2.50269552	0.00000000
H	25.72941774	2.50268470	0.00000000
H	23.27810242	-2.50282588	0.00000000
H	23.27810729	2.50282029	0.00000000
H	20.82815649	-2.50254331	0.00000000
H	20.82816055	2.50254222	0.00000000
H	18.37850699	-2.50222452	0.00000000
H	18.37851025	2.50222695	0.00000000
H	15.92861808	-2.50202287	0.00000000
H	15.92862066	2.50202802	0.00000000
H	13.47835930	-2.50194784	0.00000000
H	13.47836138	2.50195521	0.00000000
H	11.02781858	-2.50195071	0.00000000
H	11.02782021	2.50195992	0.00000000
H	8.57716063	-2.50198214	0.00000000
H	8.57716179	2.50199275	0.00000000
H	6.12649609	-2.50201406	0.00000000
H	6.12649680	2.50202556	0.00000000
H	3.67587106	-2.50203439	0.00000000
H	3.67587138	2.50204636	0.00000000
H	1.22528530	-2.50204350	0.00000000
H	1.22528538	2.50205560	0.00000000
H	-1.22528523	-2.50204351	0.00000000
H	-1.22528535	2.50205559	0.00000000
H	-3.67587099	-2.50203445	0.00000000
H	-3.67587135	2.50204632	0.00000000
H	-6.12649600	-2.50201414	0.00000000
H	-6.12649671	2.50202552	0.00000000
H	-8.57716053	-2.50198223	0.00000000
H	-8.57716171	2.50199270	0.00000000
H	-11.02781851	-2.50195079	0.00000000

H	-11.02782012	2.50195987	0.00000000
H	-13.47835928	-2.50194791	0.00000000
H	-13.47836137	2.50195518	0.00000000
H	-15.92861811	-2.50202294	0.00000000
H	-15.92862071	2.50202798	0.00000000
H	-18.37850708	-2.50222460	0.00000000
H	-18.37851032	2.50222688	0.00000000
H	-20.82815663	-2.50254336	0.00000000
H	-20.82816064	2.50254216	0.00000000
H	-23.27810256	-2.50282587	0.00000000
H	-23.27810734	2.50282027	0.00000000
H	-25.72941251	-2.50269548	0.00000000
H	-25.72941778	2.50268473	0.00000000
H	-28.18371373	-2.50133452	0.00000000
H	-28.18371901	2.50131839	0.00000000
H	-30.63633610	-2.50084097	0.00000000
H	-30.63634115	2.50081976	0.00000000
H	-32.78156130	-1.24964777	0.00000000
H	-32.78156379	1.24962232	0.00000000

26-acene (triplet), E = -4036.1090177581

C	31.82853289	-0.70802185	0.00000000
C	31.82853536	0.70798741	0.00000000
C	30.64521038	-1.40193514	0.00000000
C	30.64521518	1.40190499	0.00000000
C	29.40152730	-0.72164792	0.00000000
C	29.40152977	0.72162215	0.00000000
C	28.18366489	-1.40106067	0.00000000
C	28.18366940	1.40103938	0.00000000
C	26.95776649	-0.72518442	0.00000000
C	26.95776889	0.72516733	0.00000000
C	25.72987876	-1.40254814	0.00000000
C	25.72988303	1.40253551	0.00000000
C	24.50923988	-0.72706278	0.00000000
C	24.50924213	0.72705393	0.00000000
C	23.27913256	-1.40267492	0.00000000
C	23.27913658	1.40267006	0.00000000
C	22.05821744	-0.72769417	0.00000000
C	22.05821942	0.72769254	0.00000000
C	20.82936429	-1.40238232	0.00000000
C	20.82936807	1.40238400	0.00000000
C	19.60646691	-0.72765990	0.00000000
C	19.60646868	0.72766419	0.00000000
C	18.37956178	-1.40206215	0.00000000
C	18.37956531	1.40206905	0.00000000
C	17.15490990	-0.72740462	0.00000000
C	17.15491147	0.72741359	0.00000000
C	15.92936775	-1.40186989	0.00000000
C	15.92937097	1.40188097	0.00000000
C	14.70380744	-0.72718242	0.00000000
C	14.70380883	0.72719504	0.00000000
C	13.47882733	-1.40180658	0.00000000
C	13.47883011	1.40182091	0.00000000
C	12.25306487	-0.72707104	0.00000000
C	12.25306598	0.72708637	0.00000000
C	11.02810741	-1.40181680	0.00000000
C	11.02810964	1.40183341	0.00000000
C	9.80248422	-0.72704652	0.00000000
C	9.80248501	0.72706357	0.00000000
C	8.57735500	-1.40184722	0.00000000
C	8.57735661	1.40186508	0.00000000
C	7.35192464	-0.72706493	0.00000000
C	7.35192509	0.72708269	0.00000000
C	6.12663672	-1.40187257	0.00000000
C	6.12663768	1.40189062	0.00000000
C	4.90132372	-0.72709122	0.00000000
C	4.90132386	0.72710870	0.00000000
C	3.67596272	-1.40188524	0.00000000
C	3.67596309	1.40190250	0.00000000
C	2.45067561	-0.72710948	0.00000000
C	2.45067548	0.72712583	0.00000000
C	1.22531811	-1.40188992	0.00000000
C	1.22531804	1.40190557	0.00000000
C	0.00000066	-0.72711633	0.00000000
C	0.00000029	0.72713082	0.00000000
C	-1.22531693	-1.40189112	0.00000000
C	-1.22531730	1.40190443	0.00000000
C	-2.45067447	-0.72711169	0.00000000
C	-2.45067494	0.72712370	0.00000000
C	-3.67596194	-1.40188866	0.00000000
C	-3.67596243	1.40189920	0.00000000
C	-4.90132299	-0.72709540	0.00000000
C	-4.90132347	0.72710463	0.00000000
C	-6.12663663	-1.40187785	0.00000000

C	-6.12663708	1.40188549	0.00000000
C	-7.35192446	-0.72707064	0.00000000
C	-7.35192489	0.72707708	0.00000000
C	-8.57735559	-1.40185377	0.00000000
C	-8.57735595	1.40185863	0.00000000
C	-9.80248448	-0.72705321	0.00000000
C	-9.80248484	0.72705692	0.00000000
C	-11.02810846	-1.40182402	0.00000000
C	-11.02810875	1.40182619	0.00000000
C	-12.25306530	-0.72707821	0.00000000
C	-12.25306564	0.72707918	0.00000000
C	-13.47882857	-1.40181395	0.00000000
C	-13.47882884	1.40181345	0.00000000
C	-14.70380785	-0.72718958	0.00000000
C	-14.70380820	0.72718782	0.00000000
C	-15.92936897	-1.40187698	0.00000000
C	-15.92936929	1.40187380	0.00000000
C	-17.15491018	-0.72741130	0.00000000
C	-17.15491058	0.72740686	0.00000000
C	-18.37956292	-1.40206846	0.00000000
C	-18.37956340	1.40206271	0.00000000
C	-19.60646718	-0.72766553	0.00000000
C	-19.60646765	0.72765857	0.00000000
C	-20.82936551	-1.40238725	0.00000000
C	-20.82936619	1.40237911	0.00000000
C	-22.05821800	-0.72769790	0.00000000
C	-22.05821844	0.72768889	0.00000000
C	-23.27913412	-1.40267751	0.00000000
C	-23.27913495	1.40266762	0.00000000
C	-24.50924099	-0.72706357	0.00000000
C	-24.50924135	0.72705327	0.00000000
C	-25.72988085	-1.40254734	0.00000000
C	-25.72988173	1.40253649	0.00000000
C	-26.95776815	-0.72518146	0.00000000
C	-26.95776845	0.72517042	0.00000000
C	-28.18366754	-1.40105583	0.00000000
C	-28.18366836	1.40104440	0.00000000
C	-29.40152935	-0.72164093	0.00000000
C	-29.40152965	0.72162925	0.00000000
C	-30.64521357	-1.40192618	0.00000000
C	-30.64521419	1.40191409	0.00000000
C	-31.82853518	-0.70801086	0.00000000
C	-31.82853545	0.70799846	0.00000000
H	32.78274983	-1.24964026	0.00000000
H	32.78275417	1.24960256	0.00000000
H	30.63739130	-2.50075526	0.00000000
H	30.63739987	2.50072521	0.00000000
H	28.18467847	-2.50126186	0.00000000
H	28.18468661	2.50124066	0.00000000
H	25.73033192	-2.50263297	0.00000000
H	25.73033967	2.50262045	0.00000000
H	23.27902215	-2.50277414	0.00000000
H	23.27902943	2.50276940	0.00000000
H	20.82906217	-2.50250540	0.00000000
H	20.82906889	2.50250719	0.00000000
H	18.37932586	-2.50220378	0.00000000
H	18.37933193	2.50221081	0.00000000
H	15.92927937	-2.50202090	0.00000000
H	15.92928475	2.50203214	0.00000000
H	13.47884330	-2.50196044	0.00000000
H	13.47884783	2.50197498	0.00000000
H	11.02815223	-2.50196951	0.00000000
H	11.02815581	2.50198638	0.00000000
H	8.57738776	-2.50199795	0.00000000
H	8.57739029	2.50201608	0.00000000
H	6.12664918	-2.50202156	0.00000000
H	6.12665065	2.50203986	0.00000000
H	3.67596319	-2.50203336	0.00000000
H	3.67596371	2.50205082	0.00000000
H	1.22531698	-2.50203776	0.00000000
H	1.22531677	2.50205355	0.00000000
H	-1.22531554	-2.50203902	0.00000000
H	-1.22531633	2.50205238	0.00000000
H	-3.67596222	-2.50203694	0.00000000
H	-3.67596327	2.50204746	0.00000000
H	-6.12664904	-2.50202705	0.00000000
H	-6.12665008	2.50203462	0.00000000
H	-8.57738848	-2.50200472	0.00000000
H	-8.57738943	2.50200949	0.00000000
H	-11.02815361	-2.50197691	0.00000000
H	-11.02815453	2.50197899	0.00000000
H	-13.47884508	-2.50196792	0.00000000
H	-13.47884601	2.50196737	0.00000000

H	-15.92928135	-2.50202805	0.00000000
H	-15.92928233	2.50202485	0.00000000
H	-18.37932797	-2.50221015	0.00000000
H	-18.37932910	2.50220442	0.00000000
H	-20.82906460	-2.50251041	0.00000000
H	-20.82906588	2.50250230	0.00000000
H	-23.27902511	-2.50277686	0.00000000
H	-23.27902646	2.50276698	0.00000000
H	-25.73033549	-2.50263232	0.00000000
H	-25.73033690	2.50262145	0.00000000
H	-28.18468265	-2.50125715	0.00000000
H	-28.18468402	2.50124569	0.00000000
H	-30.63739614	-2.50074642	0.00000000
H	-30.63739724	2.50073429	0.00000000
H	-32.78275305	-1.24962792	0.00000000
H	-32.78275354	1.24961509	0.00000000

28-acene (singlet), E = -4340.5952268175

C	34.27780045	-0.70812187	0.00000000
C	34.27780212	0.70809859	0.00000000
C	33.09467720	-1.40202174	0.00000000
C	33.09468052	1.40200128	0.00000000
C	31.85079791	-0.72173010	0.00000000
C	31.85079961	0.72171254	0.00000000
C	30.63322604	-1.40113518	0.00000000
C	30.63322916	1.40112052	0.00000000
C	29.40715329	-0.72522320	0.00000000
C	29.40715481	0.72521102	0.00000000
C	28.17947358	-1.40261383	0.00000000
C	28.17947634	1.40260438	0.00000000
C	26.95886293	-0.72708223	0.00000000
C	26.95886423	0.72707495	0.00000000
C	25.72872902	-1.40273003	0.00000000
C	25.72873137	1.40272505	0.00000000
C	24.50809977	-0.72773383	0.00000000
C	24.50810087	0.72773071	0.00000000
C	23.27899701	-1.40242130	0.00000000
C	23.27899895	1.40242009	0.00000000
C	22.05652585	-0.72773862	0.00000000
C	22.05652675	0.72773886	0.00000000
C	20.82930622	-1.40208294	0.00000000
C	20.82930772	1.40208476	0.00000000
C	19.60503014	-0.72750956	0.00000000
C	19.60503081	0.72751242	0.00000000
C	18.37927693	-1.40187217	0.00000000
C	18.37927807	1.40187628	0.00000000
C	17.15392146	-0.72728509	0.00000000
C	17.15392194	0.72728998	0.00000000
C	15.92890071	-1.40179237	0.00000000
C	15.92890154	1.40179819	0.00000000
C	14.70317090	-0.72715196	0.00000000
C	14.70317123	0.72715837	0.00000000
C	13.47831550	-1.40179522	0.00000000
C	13.47831610	1.40180232	0.00000000
C	12.25262708	-0.72710696	0.00000000
C	12.25262730	0.72711455	0.00000000
C	11.02765907	-1.40182882	0.00000000
C	11.02765952	1.40183685	0.00000000
C	9.80215070	-0.72711202	0.00000000
C	9.80215089	0.72712047	0.00000000
C	8.57701271	-1.40186093	0.00000000
C	8.57701310	1.40186969	0.00000000
C	7.35166260	-0.72713467	0.00000000
C	7.35166281	0.72714383	0.00000000
C	6.12640332	-1.40188051	0.00000000
C	6.12640370	1.40188993	0.00000000
C	4.90113655	-0.72715533	0.00000000
C	4.90113677	0.72716507	0.00000000
C	3.67582816	-1.40188814	0.00000000
C	3.67582845	1.40189815	0.00000000
C	2.45057699	-0.72716766	0.00000000
C	2.45057713	0.72717781	0.00000000
C	1.22527373	-1.40188993	0.00000000
C	1.22527382	1.40190027	0.00000000
C	-0.00000019	-0.72717160	0.00000000
C	-0.00000019	0.72718186	0.00000000
C	-1.22527407	-1.40188994	0.00000000
C	-1.22527421	1.40190023	0.00000000
C	-2.45057731	-0.72716771	0.00000000
C	-2.45057748	0.72717773	0.00000000
C	-3.67582840	-1.40188818	0.00000000
C	-3.67582874	1.40189801	0.00000000
C	-4.90113673	-0.72715540	0.00000000
C	-4.90113698	0.72716494	0.00000000

C	-6.12640341	-1.40188057	0.00000000
C	-6.12640383	1.40188974	0.00000000
C	-7.35166261	-0.72713477	0.00000000
C	-7.35166284	0.72714365	0.00000000
C	-8.57701264	-1.40186104	0.00000000
C	-8.57701306	1.40186949	0.00000000
C	-9.80215060	-0.72711215	0.00000000
C	-9.80215080	0.72712029	0.00000000
C	-11.02765894	-1.40182898	0.00000000
C	-11.02765941	1.40183666	0.00000000
C	-12.25262697	-0.72710716	0.00000000
C	-12.25262721	0.72711438	0.00000000
C	-13.47831544	-1.40179544	0.00000000
C	-13.47831604	1.40180218	0.00000000
C	-14.70317090	-0.72715216	0.00000000
C	-14.70317123	0.72715823	0.00000000
C	-15.92890079	-1.40179258	0.00000000
C	-15.92890161	1.40179807	0.00000000
C	-17.15392162	-0.72728528	0.00000000
C	-17.15392210	0.72728985	0.00000000
C	-18.37927718	-1.40187235	0.00000000
C	-18.37927830	1.40187615	0.00000000
C	-19.60503044	-0.72750970	0.00000000
C	-19.60503111	0.72751230	0.00000000
C	-20.82930656	-1.40208306	0.00000000
C	-20.82930804	1.40208462	0.00000000
C	-22.05652618	-0.72773872	0.00000000
C	-22.05652706	0.72773874	0.00000000
C	-23.27899731	-1.40242135	0.00000000
C	-23.27899919	1.40241997	0.00000000
C	-24.50809997	-0.72773385	0.00000000
C	-24.50810105	0.72773061	0.00000000
C	-25.72872914	-1.40272999	0.00000000
C	-25.72873140	1.40272495	0.00000000
C	-26.95886290	-0.72708217	0.00000000
C	-26.95886416	0.72707492	0.00000000
C	-28.17947345	-1.40261369	0.00000000
C	-28.17947611	1.40260433	0.00000000
C	-29.40715302	-0.72522307	0.00000000
C	-29.40715448	0.72521104	0.00000000
C	-30.63322568	-1.40113499	0.00000000
C	-30.63322870	1.40112055	0.00000000
C	-31.85079743	-0.72172991	0.00000000
C	-31.85079908	0.72171266	0.00000000
C	-33.09467667	-1.40202147	0.00000000
C	-33.09467988	1.40200142	0.00000000
C	-34.27779984	-0.70812160	0.00000000
C	-34.27780145	0.70809881	0.00000000
H	35.23206937	-1.24964997	0.00000000
H	35.23207232	1.24962445	0.00000000
H	33.08685975	-2.50084221	0.00000000
H	33.08686560	2.50082182	0.00000000
H	30.63423188	-2.50133640	0.00000000
H	30.63423733	2.50132188	0.00000000
H	28.17993126	-2.50269857	0.00000000
H	28.17993624	2.50268929	0.00000000
H	25.72862556	-2.50282987	0.00000000
H	25.72862979	2.50282508	0.00000000
H	23.27868649	-2.50254666	0.00000000
H	23.27868991	2.50254563	0.00000000
H	20.82904347	-2.50222802	0.00000000
H	20.82904615	2.50223002	0.00000000
H	18.37915618	-2.50202826	0.00000000
H	18.37915827	2.50203251	0.00000000
H	15.92889727	-2.50195220	0.00000000
H	15.92889885	2.50195814	0.00000000
H	13.47836268	-2.50195441	0.00000000
H	13.47836389	2.50196158	0.00000000
H	11.02770710	-2.50198588	0.00000000
H	11.02770802	2.50199393	0.00000000
H	8.57704054	-2.50201592	0.00000000
H	8.57704128	2.50202466	0.00000000
H	6.12641220	-2.50203404	0.00000000
H	6.12641278	2.50204346	0.00000000
H	3.67582786	-2.50204097	0.00000000
H	3.67582824	2.50205103	0.00000000
H	1.22527272	-2.50204249	0.00000000
H	1.22527280	2.50205292	0.00000000
H	-1.22527293	-2.50204248	0.00000000
H	-1.22527314	2.50205286	0.00000000
H	-3.67582808	-2.50204096	0.00000000
H	-3.67582854	2.50205085	0.00000000
H	-6.12641228	-2.50203405	0.00000000

H	-6.12641293	2.50204322	0.00000000
H	-8.57704049	-2.50201599	0.00000000
H	-8.57704125	2.50202442	0.00000000
H	-11.02770698	-2.50198604	0.00000000
H	-11.02770794	2.50199373	0.00000000
H	-13.47836265	-2.50195465	0.00000000
H	-13.47836384	2.50196144	0.00000000
H	-15.92889737	-2.50195244	0.00000000
H	-15.92889892	2.50195804	0.00000000
H	-18.37915643	-2.50202846	0.00000000
H	-18.37915847	2.50203240	0.00000000
H	-20.82904380	-2.50222814	0.00000000
H	-20.82904644	2.50222987	0.00000000
H	-23.27868679	-2.50254668	0.00000000
H	-23.27869012	2.50254547	0.00000000
H	-25.72862571	-2.50282976	0.00000000
H	-25.72862977	2.50282491	0.00000000
H	-28.17993115	-2.50269836	0.00000000
H	-28.17993600	2.50268916	0.00000000
H	-30.63423156	-2.50133615	0.00000000
H	-30.63423684	2.50132184	0.00000000
H	-33.08685926	-2.50084189	0.00000000
H	-33.08686492	2.50082192	0.00000000
H	-35.23206883	-1.24964967	0.00000000
H	-35.23207166	1.24962473	0.00000000

28-acene (triplet), E = -4340.5923151405

C	34.27893719	-0.70801884	0.00000000
C	34.27893758	0.70801512	0.00000000
C	33.09564493	-1.40193612	0.00000000
C	33.09564557	1.40193307	0.00000000
C	31.85193697	-0.72164907	0.00000000
C	31.85193741	0.72164684	0.00000000
C	30.63411570	-1.40106399	0.00000000
C	30.63411630	1.40106254	0.00000000
C	29.40819337	-0.72518258	0.00000000
C	29.40819394	0.72518213	0.00000000
C	28.18033815	-1.40255440	0.00000000
C	28.18033874	1.40255482	0.00000000
C	26.95970257	-0.72706065	0.00000000
C	26.95970311	0.72706195	0.00000000
C	25.72959566	-1.40268329	0.00000000
C	25.72959629	1.40268538	0.00000000
C	24.50872035	-0.72769713	0.00000000
C	24.50872068	0.72769971	0.00000000
C	23.27983550	-1.40239015	0.00000000
C	23.27983618	1.40239317	0.00000000
C	22.05699822	-0.72767063	0.00000000
C	22.05699832	0.72767372	0.00000000
C	20.83005201	-1.40207023	0.00000000
C	20.83005272	1.40207338	0.00000000
C	19.60545321	-0.72742235	0.00000000
C	19.60545315	0.72742525	0.00000000
C	18.37988440	-1.40187840	0.00000000
C	18.37988516	1.40188110	0.00000000
C	17.15435378	-0.72720220	0.00000000
C	17.15435365	0.72720451	0.00000000
C	15.92936870	-1.40181373	0.00000000
C	15.92936947	1.40181563	0.00000000
C	14.70361148	-0.72708832	0.00000000
C	14.70361132	0.72708977	0.00000000
C	13.47867341	-1.40182360	0.00000000
C	13.47867421	1.40182454	0.00000000
C	12.25303961	-0.72706286	0.00000000
C	12.25303948	0.72706342	0.00000000
C	11.02794009	-1.40185612	0.00000000
C	11.02794099	1.40185618	0.00000000
C	9.80249685	-0.72707886	0.00000000
C	9.80249679	0.72707869	0.00000000
C	8.57723642	-1.40188200	0.00000000
C	8.57723750	1.40188146	0.00000000
C	7.35192040	-0.72710271	0.00000000
C	7.35192046	0.72710216	0.00000000
C	6.12657270	-1.40189427	0.00000000
C	6.12657397	1.40189352	0.00000000
C	4.90130220	-0.72711875	0.00000000
C	4.90130237	0.72711820	0.00000000
C	3.67593570	-1.40189621	0.00000000
C	3.67593707	1.40189562	0.00000000
C	2.45065660	-0.72712574	0.00000000
C	2.45065685	0.72712541	0.00000000
C	1.22531029	-1.40189499	0.00000000
C	1.22531172	1.40189476	0.00000000
C	-0.00000042	-0.72712729	0.00000000

C	-0.00000016	0.72712734	0.00000000
C	-1.22531232	-1.40189478	0.00000000
C	-1.22531089	1.40189502	0.00000000
C	-2.45065739	-0.72712538	0.00000000
C	-2.45065716	0.72712579	0.00000000
C	-3.67593760	-1.40189569	0.00000000
C	-3.67593622	1.40189625	0.00000000
C	-4.90130282	-0.72711821	0.00000000
C	-4.90130267	0.72711878	0.00000000
C	-6.12657439	-1.40189362	0.00000000
C	-6.12657310	1.40189429	0.00000000
C	-7.35192083	-0.72710218	0.00000000
C	-7.35192077	0.72710273	0.00000000
C	-8.57723782	-1.40188152	0.00000000
C	-8.57723668	1.40188200	0.00000000
C	-9.80249708	-0.72707869	0.00000000
C	-9.80249712	0.72707888	0.00000000
C	-11.02794123	-1.40185620	0.00000000
C	-11.02794028	1.40185609	0.00000000
C	-12.25303968	-0.72706339	0.00000000
C	-12.25303980	0.72706286	0.00000000
C	-13.47867439	-1.40182450	0.00000000
C	-13.47867355	1.40182353	0.00000000
C	-14.70361147	-0.72708970	0.00000000
C	-14.70361161	0.72708832	0.00000000
C	-15.92936960	-1.40181553	0.00000000
C	-15.92936881	1.40181368	0.00000000
C	-17.15435371	-0.72720438	0.00000000
C	-17.15435383	0.72720226	0.00000000
C	-18.37988520	-1.40188097	0.00000000
C	-18.37988447	1.40187839	0.00000000
C	-19.60545315	-0.72742512	0.00000000
C	-19.60545319	0.72742241	0.00000000
C	-20.83005270	-1.40207325	0.00000000
C	-20.83005200	1.40207025	0.00000000
C	-22.05699823	-0.72767358	0.00000000
C	-22.05699809	0.72767073	0.00000000
C	-23.27983603	-1.40239306	0.00000000
C	-23.27983538	1.40239024	0.00000000
C	-24.50872049	-0.72769958	0.00000000
C	-24.50872013	0.72769725	0.00000000
C	-25.72959601	-1.40268528	0.00000000
C	-25.72959537	1.40268342	0.00000000
C	-26.95970279	-0.72706181	0.00000000
C	-26.95970221	0.72706079	0.00000000
C	-28.18033835	-1.40255470	0.00000000
C	-28.18033767	1.40255459	0.00000000
C	-29.40819351	-0.72518192	0.00000000
C	-29.40819288	0.72518282	0.00000000
C	-30.63411581	-1.40106233	0.00000000
C	-30.63411511	1.40106430	0.00000000
C	-31.85193686	-0.72164652	0.00000000
C	-31.85193634	0.72164939	0.00000000
C	-33.09564499	-1.40193272	0.00000000
C	-33.09564422	1.40193651	0.00000000
C	-34.27893695	-0.70801470	0.00000000
C	-34.27893649	0.70801925	0.00000000
H	35.23315819	-1.24962786	0.00000000
H	35.23315887	1.24962362	0.00000000
H	33.08783716	-2.50075664	0.00000000
H	33.08783848	2.50075360	0.00000000
H	30.63513130	-2.50126571	0.00000000
H	30.63513270	2.50126425	0.00000000
H	28.18079140	-2.50263970	0.00000000
H	28.18079268	2.50264010	0.00000000
H	25.72948523	-2.50278297	0.00000000
H	25.72948637	2.50278503	0.00000000
H	23.27953335	-2.50251408	0.00000000
H	23.27953431	2.50251708	0.00000000
H	20.82981522	-2.50221251	0.00000000
H	20.82981602	2.50221563	0.00000000
H	18.37979249	-2.50203044	0.00000000
H	18.37979322	2.50203311	0.00000000
H	15.92938176	-2.50196857	0.00000000
H	15.92938245	2.50197043	0.00000000
H	13.47872069	-2.50197733	0.00000000
H	13.47872142	2.50197821	0.00000000
H	11.02797677	-2.50200770	0.00000000
H	11.02797766	2.50200767	0.00000000
H	8.57725032	-2.50203184	0.00000000
H	8.57725151	2.50203118	0.00000000
H	6.12657091	-2.50204315	0.00000000
H	6.12657239	2.50204230	0.00000000

H	3.67592953	-2.50204487	0.00000000
H	3.67593115	2.50204422	0.00000000
H	1.22530731	-2.50204368	0.00000000
H	1.22530902	2.50204341	0.00000000
H	-1.22530967	-2.50204347	0.00000000
H	-1.22530797	2.50204368	0.00000000
H	-3.67593169	-2.50204434	0.00000000
H	-3.67593008	2.50204491	0.00000000
H	-6.12657278	-2.50204246	0.00000000
H	-6.12657127	2.50204316	0.00000000
H	-8.57725176	-2.50203129	0.00000000
H	-8.57725052	2.50203182	0.00000000
H	-11.02797783	-2.50200770	0.00000000
H	-11.02797691	2.50200763	0.00000000
H	-13.47872155	-2.50197816	0.00000000
H	-13.47872078	2.50197720	0.00000000
H	-15.92938260	-2.50197030	0.00000000
H	-15.92938183	2.50196844	0.00000000
H	-18.37979331	-2.50203295	0.00000000
H	-18.37979261	2.50203035	0.00000000
H	-20.82981605	-2.50221549	0.00000000
H	-20.82981529	2.50221247	0.00000000
H	-23.27953421	-2.50251698	0.00000000
H	-23.27953330	2.50251415	0.00000000
H	-25.72948612	-2.50278497	0.00000000
H	-25.72948499	2.50278310	0.00000000
H	-28.18079231	-2.50264002	0.00000000
H	-28.18079088	2.50263992	0.00000000
H	-30.63513226	-2.50126408	0.00000000
H	-30.63513068	2.50126604	0.00000000
H	-33.08783792	-2.50075327	0.00000000
H	-33.08783641	2.50075704	0.00000000
H	-35.23315828	-1.24962319	0.00000000
H	-35.23315748	1.24962832	0.00000000

30-acene (singlet), E = -4645.0782858828

C	36.72830544	-0.70811831	0.00000000
C	36.72830653	0.70810151	0.00000000
C	35.54518203	-1.40202195	0.00000000
C	35.54518420	1.40200702	0.00000000
C	34.30130634	-0.72172797	0.00000000
C	34.30130741	0.72171497	0.00000000
C	33.08373392	-1.40113631	0.00000000
C	33.08373604	1.40112514	0.00000000
C	31.85766221	-0.72522151	0.00000000
C	31.85766333	0.72521225	0.00000000
C	30.62998547	-1.40261479	0.00000000
C	30.62998752	1.40260735	0.00000000
C	29.40937451	-0.72708138	0.00000000
C	29.40937556	0.72707552	0.00000000
C	28.17924478	-1.40273175	0.00000000
C	28.17924645	1.40272764	0.00000000
C	26.95861430	-0.72773301	0.00000000
C	26.95861500	0.72773001	0.00000000
C	25.72951583	-1.40242479	0.00000000
C	25.72951698	1.40242311	0.00000000
C	24.50704450	-0.72773829	0.00000000
C	24.50704496	0.72773745	0.00000000
C	23.27982777	-1.40208634	0.00000000
C	23.27982859	1.40208635	0.00000000
C	22.05555273	-0.72750954	0.00000000
C	22.05555308	0.72751019	0.00000000
C	20.82980197	-1.40187599	0.00000000
C	20.82980255	1.40187723	0.00000000
C	19.60444885	-0.72728653	0.00000000
C	19.60444910	0.72728818	0.00000000
C	18.37942956	-1.40179749	0.00000000
C	18.37942997	1.40179963	0.00000000
C	17.15370173	-0.72715380	0.00000000
C	17.15370189	0.72715622	0.00000000
C	15.92884908	-1.40179956	0.00000000
C	15.92884944	1.40180235	0.00000000
C	14.70316187	-0.72710809	0.00000000
C	14.70316204	0.72711134	0.00000000
C	13.47819781	-1.40183338	0.00000000
C	13.47819837	1.40183702	0.00000000
C	12.25268985	-0.72711400	0.00000000
C	12.25269024	0.72711831	0.00000000
C	11.02755574	-1.40186580	0.00000000
C	11.02755660	1.40187068	0.00000000
C	9.80220690	-0.72713495	0.00000000
C	9.80220746	0.72714066	0.00000000
C	8.57694990	-1.40188399	0.00000000
C	8.57695092	1.40189057	0.00000000

C	7.35168920	-0.72715344	0.00000000
C	7.35168976	0.72716076	0.00000000
C	6.12637553	-1.40188984	0.00000000
C	6.12637645	1.40189817	0.00000000
C	4.90114027	-0.72716372	0.00000000
C	4.90114065	0.72717265	0.00000000
C	3.67581934	-1.40188869	0.00000000
C	3.67581993	1.40189843	0.00000000
C	2.45057250	-0.72716765	0.00000000
C	2.45057266	0.72717775	0.00000000
C	1.22527064	-1.40188663	0.00000000
C	1.22527082	1.40189707	0.00000000
C	-0.00000271	-0.72716846	0.00000000
C	-0.00000270	0.72717893	0.00000000
C	-1.22527588	-1.40188649	0.00000000
C	-1.22527607	1.40189687	0.00000000
C	-2.45057722	-0.72716747	0.00000000
C	-2.45057738	0.72717747	0.00000000
C	-3.67582327	-1.40188828	0.00000000
C	-3.67582384	1.40189794	0.00000000
C	-4.90114317	-0.72716337	0.00000000
C	-4.90114354	0.72717226	0.00000000
C	-6.12637731	-1.40188928	0.00000000
C	-6.12637821	1.40189759	0.00000000
C	-7.35168985	-0.72715307	0.00000000
C	-7.35169041	0.72716039	0.00000000
C	-8.57694953	-1.40188352	0.00000000
C	-8.57695055	1.40189010	0.00000000
C	-9.80220573	-0.72713472	0.00000000
C	-9.80220629	0.72714043	0.00000000
C	-11.02755403	-1.40186560	0.00000000
C	-11.02755489	1.40187049	0.00000000
C	-12.25268794	-0.72711398	0.00000000
C	-12.25268832	0.72711830	0.00000000
C	-13.47819601	-1.40183351	0.00000000
C	-13.47819656	1.40183717	0.00000000
C	-14.70316050	-0.72710825	0.00000000
C	-14.70316069	0.72711157	0.00000000
C	-15.92884838	-1.40179989	0.00000000
C	-15.92884876	1.40180277	0.00000000
C	-17.15370189	-0.72715409	0.00000000
C	-17.15370205	0.72715654	0.00000000
C	-18.37943062	-1.40179791	0.00000000
C	-18.37943107	1.40180007	0.00000000
C	-19.60445078	-0.72728681	0.00000000
C	-19.60445105	0.72728844	0.00000000
C	-20.82980461	-1.40187628	0.00000000
C	-20.82980522	1.40187748	0.00000000
C	-22.05555581	-0.72750965	0.00000000
C	-22.05555616	0.72751026	0.00000000
C	-23.27983096	-1.40208633	0.00000000
C	-23.27983179	1.40208628	0.00000000
C	-24.50704744	-0.72773819	0.00000000
C	-24.50704788	0.72773726	0.00000000
C	-25.72951815	-1.40242447	0.00000000
C	-25.72951932	1.40242267	0.00000000
C	-26.95861575	-0.72773274	0.00000000
C	-26.95861644	0.72772958	0.00000000
C	-28.17924512	-1.40273120	0.00000000
C	-28.17924674	1.40272697	0.00000000
C	-29.40937362	-0.72708097	0.00000000
C	-29.40937464	0.72707505	0.00000000
C	-30.62998333	-1.40261413	0.00000000
C	-30.62998534	1.40260667	0.00000000
C	-31.85765887	-0.72522107	0.00000000
C	-31.85765999	0.72521183	0.00000000
C	-33.08372955	-1.40113567	0.00000000
C	-33.08373166	1.40112453	0.00000000
C	-34.30130112	-0.72172760	0.00000000
C	-34.30130217	0.72171462	0.00000000
C	-35.54517606	-1.40202146	0.00000000
C	-35.54517819	1.40200657	0.00000000
C	-36.72829899	-0.70811807	0.00000000
C	-36.72830008	0.70810136	0.00000000
H	37.68257308	-1.24964515	0.00000000
H	37.68257501	1.24962688	0.00000000
H	35.53736566	-2.50084212	0.00000000
H	35.53736955	2.50082721	0.00000000
H	33.08474059	-2.50133725	0.00000000
H	33.08474439	2.50132611	0.00000000
H	30.63044396	-2.50269945	0.00000000
H	30.63044739	2.50269212	0.00000000
H	28.17913958	-2.50283148	0.00000000

H	28.17914249	2.50282761	0.00000000
H	25.72920393	-2.50254980	0.00000000
H	25.72920615	2.50254836	0.00000000
H	23.27956563	-2.50223112	0.00000000
H	23.27956717	2.50223129	0.00000000
H	20.82968260	-2.50203159	0.00000000
H	20.82968360	2.50203295	0.00000000
H	18.37942627	-2.50195671	0.00000000
H	18.37942704	2.50195890	0.00000000
H	15.92889848	-2.50195815	0.00000000
H	15.92889930	2.50196090	0.00000000
H	13.47824762	-2.50198973	0.00000000
H	13.47824870	2.50199324	0.00000000
H	11.02758409	-2.50202010	0.00000000
H	11.02758550	2.50202486	0.00000000
H	8.57695673	-2.50203691	0.00000000
H	8.57695837	2.50204349	0.00000000
H	6.12637068	-2.50204210	0.00000000
H	6.12637231	2.50205056	0.00000000
H	3.67581273	-2.50204088	0.00000000
H	3.67581391	2.50205081	0.00000000
H	1.22526797	-2.50203882	0.00000000
H	1.22526836	2.50204948	0.00000000
H	-1.22527297	-2.50203853	0.00000000
H	-1.22527342	2.50204913	0.00000000
H	-3.67581653	-2.50204008	0.00000000
H	-3.67581767	2.50204993	0.00000000
H	-6.12637246	-2.50204107	0.00000000
H	-6.12637406	2.50204950	0.00000000
H	-8.57695648	-2.50203604	0.00000000
H	-8.57695812	2.50204262	0.00000000
H	-11.02758259	-2.50201971	0.00000000
H	-11.02758399	2.50202449	0.00000000
H	-13.47824603	-2.50198994	0.00000000
H	-13.47824705	2.50199348	0.00000000
H	-15.92889787	-2.50195876	0.00000000
H	-15.92889872	2.50196159	0.00000000
H	-18.37942729	-2.50195745	0.00000000
H	-18.37942812	2.50195967	0.00000000
H	-20.82968507	-2.50203206	0.00000000
H	-20.82968611	2.50203339	0.00000000
H	-23.27956859	-2.50223101	0.00000000
H	-23.27957016	2.50223113	0.00000000
H	-25.72920604	-2.50254910	0.00000000
H	-25.72920832	2.50254753	0.00000000
H	-28.17913986	-2.50283037	0.00000000
H	-28.17914267	2.50282637	0.00000000
H	-30.63044190	-2.50269819	0.00000000
H	-30.63044525	2.50269085	0.00000000
H	-33.08473634	-2.50133611	0.00000000
H	-33.08474013	2.50132499	0.00000000
H	-35.53735969	-2.50084124	0.00000000
H	-35.53736350	2.50082639	0.00000000
H	-37.68256641	-1.24964475	0.00000000
H	-37.68256832	1.24962660	0.00000000

30-acene (triplet), E = -4645.0755784965

C	36.72934773	-0.70803264	0.00000000
C	36.72934804	0.70802554	0.00000000
C	35.54607820	-1.40195097	0.00000000
C	35.54607895	1.40194438	0.00000000
C	34.30235148	-0.72166086	0.00000000
C	34.30235171	0.72165471	0.00000000
C	33.08456350	-1.40107749	0.00000000
C	33.08456430	1.40107176	0.00000000
C	31.85862304	-0.72518946	0.00000000
C	31.85862311	0.72518398	0.00000000
C	30.63079435	-1.40256653	0.00000000
C	30.63079511	1.40256133	0.00000000
C	29.41016272	-0.72706601	0.00000000
C	29.41016278	0.72706110	0.00000000
C	28.18005619	-1.40269482	0.00000000
C	28.18005683	1.40269017	0.00000000
C	26.95921302	-0.72770438	0.00000000
C	26.95921327	0.72770031	0.00000000
C	25.73030371	-1.40240094	0.00000000
C	25.73030414	1.40239726	0.00000000
C	24.50751499	-0.72768181	0.00000000
C	24.50751541	0.72767894	0.00000000
C	23.28053621	-1.40207737	0.00000000
C	23.28053641	1.40207515	0.00000000
C	22.05598059	-0.72743509	0.00000000
C	22.05598111	0.72743381	0.00000000
C	20.83039071	-1.40188205	0.00000000

C	20.83039071	1.40188158	0.00000000
C	19.60488492	-0.72721409	0.00000000
C	19.60488548	0.72721464	0.00000000
C	18.37989703	-1.40181475	0.00000000
C	18.37989683	1.40181614	0.00000000
C	17.15414549	-0.72709638	0.00000000
C	17.15414605	0.72709880	0.00000000
C	15.92922099	-1.40182135	0.00000000
C	15.92922060	1.40182455	0.00000000
C	14.70358216	-0.72706661	0.00000000
C	14.70358265	0.72707070	0.00000000
C	13.47850374	-1.40185298	0.00000000
C	13.47850316	1.40185781	0.00000000
C	12.25305252	-0.72708167	0.00000000
C	12.25305288	0.72708721	0.00000000
C	11.02781376	-1.40187992	0.00000000
C	11.02781294	1.40188602	0.00000000
C	9.80249151	-0.72710418	0.00000000
C	9.80249167	0.72711064	0.00000000
C	8.57716350	-1.40189269	0.00000000
C	8.57716244	1.40189937	0.00000000
C	7.35189162	-0.72711935	0.00000000
C	7.35189160	0.72712612	0.00000000
C	6.12653869	-1.40189504	0.00000000
C	6.12653741	1.40190178	0.00000000
C	4.90126735	-0.72712502	0.00000000
C	4.90126717	0.72713164	0.00000000
C	3.67592319	-1.40189250	0.00000000
C	3.67592169	1.40189882	0.00000000
C	2.45063404	-0.72712564	0.00000000
C	2.45063372	0.72713161	0.00000000
C	1.22530814	-1.40189044	0.00000000
C	1.22530649	1.40189588	0.00000000
C	-0.00000043	-0.72712566	0.00000000
C	-0.00000081	0.72713064	0.00000000
C	-1.22530763	-1.40189091	0.00000000
C	-1.22530938	1.40189529	0.00000000
C	-2.45063474	-0.72712663	0.00000000
C	-2.45063513	0.72713051	0.00000000
C	-3.67592241	-1.40189389	0.00000000
C	-3.67592418	1.40189717	0.00000000
C	-4.90126769	-0.72712683	0.00000000
C	-4.90126803	0.72712963	0.00000000
C	-6.12653753	-1.40189711	0.00000000
C	-6.12653923	1.40189939	0.00000000
C	-7.35189153	-0.72712166	0.00000000
C	-7.35189178	0.72712361	0.00000000
C	-8.57716196	-1.40189510	0.00000000
C	-8.57716356	1.40189668	0.00000000
C	-9.80249112	-0.72710662	0.00000000
C	-9.80249125	0.72710807	0.00000000
C	-11.02781207	-1.40188231	0.00000000
C	-11.02781358	1.40188352	0.00000000
C	-12.25305214	-0.72708386	0.00000000
C	-12.25305214	0.72708502	0.00000000
C	-13.47850222	-1.40185490	0.00000000
C	-13.47850363	1.40185595	0.00000000
C	-14.70358198	-0.72706819	0.00000000
C	-14.70358197	0.72706923	0.00000000
C	-15.92921990	-1.40182255	0.00000000
C	-15.92922123	1.40182357	0.00000000
C	-17.15414579	-0.72709723	0.00000000
C	-17.15414575	0.72709814	0.00000000
C	-18.37989654	-1.40181508	0.00000000
C	-18.37989779	1.40181607	0.00000000
C	-19.60488567	-0.72721403	0.00000000
C	-19.60488568	0.72721487	0.00000000
C	-20.83039078	-1.40188148	0.00000000
C	-20.83039193	1.40188231	0.00000000
C	-22.05598160	-0.72743419	0.00000000
C	-22.05598169	0.72743478	0.00000000
C	-23.28053662	-1.40207603	0.00000000
C	-23.28053763	1.40207649	0.00000000
C	-24.50751587	-0.72768036	0.00000000
C	-24.50751610	0.72768034	0.00000000
C	-25.73030414	-1.40239920	0.00000000
C	-25.73030500	1.40239882	0.00000000
C	-26.95921335	-0.72770284	0.00000000
C	-26.95921381	0.72770168	0.00000000
C	-28.18005633	-1.40269324	0.00000000
C	-28.18005705	1.40269143	0.00000000
C	-29.41016231	-0.72706485	0.00000000
C	-29.41016295	0.72706205	0.00000000

C	-30.63079402	-1.40256561	0.00000000
C	-30.63079463	1.40256192	0.00000000
C	-31.85862206	-0.72518893	0.00000000
C	-31.85862269	0.72518430	0.00000000
C	-33.08456269	-1.40107725	0.00000000
C	-33.08456327	1.40107166	0.00000000
C	-34.30235023	-0.72166088	0.00000000
C	-34.30235071	0.72165451	0.00000000
C	-35.54607696	-1.40195113	0.00000000
C	-35.54607758	1.40194397	0.00000000
C	-36.72934629	-0.70803295	0.00000000
C	-36.72934668	0.70802514	0.00000000
H	37.68357361	-1.24962972	0.00000000
H	37.68357417	1.24962217	0.00000000
H	35.53826989	-2.50077104	0.00000000
H	35.53827103	2.50076445	0.00000000
H	33.08557847	-2.50127870	0.00000000
H	33.08557954	2.50127299	0.00000000
H	30.63124890	-2.50265153	0.00000000
H	30.63124996	2.50264636	0.00000000
H	28.17994472	-2.50279434	0.00000000
H	28.17994578	2.50278974	0.00000000
H	25.72999890	-2.50252467	0.00000000
H	25.72999982	2.50252104	0.00000000
H	23.28029610	-2.50221968	0.00000000
H	23.28029696	2.50221751	0.00000000
H	20.83029567	-2.50203412	0.00000000
H	20.83029647	2.50203370	0.00000000
H	18.37990725	-2.50196964	0.00000000
H	18.37990783	2.50197106	0.00000000
H	15.92926954	-2.50197511	0.00000000
H	15.92926981	2.50197835	0.00000000
H	13.47854378	-2.50200443	0.00000000
H	13.47854373	2.50200931	0.00000000
H	11.02783060	-2.50202954	0.00000000
H	11.02783011	2.50203571	0.00000000
H	8.57716281	-2.50204133	0.00000000
H	8.57716183	2.50204807	0.00000000
H	6.12653152	-2.50204337	0.00000000
H	6.12653011	2.50205016	0.00000000
H	3.67591726	-2.50204096	0.00000000
H	3.67591536	2.50204731	0.00000000
H	1.22530628	-2.50203904	0.00000000
H	1.22530408	2.50204448	0.00000000
H	-1.22530509	-2.50203948	0.00000000
H	-1.22530747	2.50204384	0.00000000
H	-3.67591595	-2.50204229	0.00000000
H	-3.67591832	2.50204551	0.00000000
H	-6.12653007	-2.50204537	0.00000000
H	-6.12653224	2.50204757	0.00000000
H	-8.57716120	-2.50204372	0.00000000
H	-8.57716312	2.50204521	0.00000000
H	-11.02782901	-2.50203195	0.00000000
H	-11.02783078	2.50203308	0.00000000
H	-13.47854250	-2.50200643	0.00000000
H	-13.47854409	2.50200742	0.00000000
H	-15.92926875	-2.50197644	0.00000000
H	-15.92927022	2.50197741	0.00000000
H	-18.37990710	-2.50197009	0.00000000
H	-18.37990842	2.50197105	0.00000000
H	-20.83029603	-2.50203367	0.00000000
H	-20.83029730	2.50203446	0.00000000
H	-23.28029661	-2.50221838	0.00000000
H	-23.28029792	2.50221879	0.00000000
H	-25.72999924	-2.50252288	0.00000000
H	-25.73000063	2.50252246	0.00000000
H	-28.17994469	-2.50279265	0.00000000
H	-28.17994609	2.50279081	0.00000000
H	-30.63124834	-2.50265048	0.00000000
H	-30.63124971	2.50264675	0.00000000
H	-33.08557741	-2.50127834	0.00000000
H	-33.08557879	2.50127273	0.00000000
H	-35.53826850	-2.50077111	0.00000000
H	-35.53826981	2.50076395	0.00000000
H	-37.68357207	-1.24962998	0.00000000
H	-37.68357273	1.24962169	0.00000000
32-acene (singlet), E = -4949.5613446400			
C	39.17880567	-0.70809239	0.00000000
C	39.17880419	0.70812461	0.00000000
C	37.99568346	-1.40200128	0.00000000
C	37.99568053	1.40203100	0.00000000
C	36.75181182	-0.72170726	0.00000000
C	36.75181033	0.72173444	0.00000000

C	35.53424038	-1.40111973	0.00000000
C	35.53423753	1.40114436	0.00000000
C	34.30817221	-0.72520548	0.00000000
C	34.30817078	0.72522772	0.00000000
C	33.08049784	-1.40260318	0.00000000
C	33.08049509	1.40262292	0.00000000
C	31.85988753	-0.72706902	0.00000000
C	31.85988616	0.72708641	0.00000000
C	30.62976369	-1.40272342	0.00000000
C	30.62976108	1.40273847	0.00000000
C	29.40913299	-0.72772479	0.00000000
C	29.40913166	0.72773759	0.00000000
C	28.18003981	-1.40242031	0.00000000
C	28.18003729	1.40243093	0.00000000
C	26.95756783	-0.72773289	0.00000000
C	26.95756652	0.72774132	0.00000000
C	25.73035591	-1.40208628	0.00000000
C	25.73035344	1.40209259	0.00000000
C	24.50608112	-0.72750715	0.00000000
C	24.50607982	0.72751133	0.00000000
C	23.28033304	-1.40187814	0.00000000
C	23.28033059	1.40188019	0.00000000
C	22.05498034	-0.72728672	0.00000000
C	22.05497908	0.72728666	0.00000000
C	20.82996271	-1.40180234	0.00000000
C	20.82996035	1.40180017	0.00000000
C	19.60423615	-0.72715749	0.00000000
C	19.60423496	0.72715335	0.00000000
C	18.37938396	-1.40180771	0.00000000
C	18.37938182	1.40180161	0.00000000
C	17.15369716	-0.72711393	0.00000000
C	17.15369610	0.72710613	0.00000000
C	15.92873474	-1.40184235	0.00000000
C	15.92873291	1.40183277	0.00000000
C	14.70322735	-0.72712075	0.00000000
C	14.70322649	0.72710979	0.00000000
C	13.47809639	-1.40187674	0.00000000
C	13.47809493	1.40186431	0.00000000
C	12.25274753	-0.72714512	0.00000000
C	12.25274692	0.72713158	0.00000000
C	11.02749418	-1.40189782	0.00000000
C	11.02749318	1.40188323	0.00000000
C	9.80223238	-0.72716462	0.00000000
C	9.80223198	0.72714930	0.00000000
C	8.57692378	-1.40190493	0.00000000
C	8.57692316	1.40188891	0.00000000
C	7.35168871	-0.72717510	0.00000000
C	7.35168846	0.72715862	0.00000000
C	6.12637030	-1.40190445	0.00000000
C	6.12636994	1.40188760	0.00000000
C	4.90112947	-0.72717822	0.00000000
C	4.90112931	0.72716107	0.00000000
C	3.67582221	-1.40190119	0.00000000
C	3.67582194	1.40188378	0.00000000
C	2.45056483	-0.72717815	0.00000000
C	2.45056469	0.72716048	0.00000000
C	1.22527405	-1.40189905	0.00000000
C	1.22527378	1.40188117	0.00000000
C	-0.00000036	-0.72717794	0.00000000
C	-0.00000052	0.72715981	0.00000000
C	-1.22527463	-1.40189931	0.00000000
C	-1.22527497	1.40188088	0.00000000
C	-2.45056546	-0.72717867	0.00000000
C	-2.45056561	0.72715991	0.00000000
C	-3.67582259	-1.40190196	0.00000000
C	-3.67582288	1.40188294	0.00000000
C	-4.90112982	-0.72717924	0.00000000
C	-4.90112992	0.72715997	0.00000000
C	-6.12637038	-1.40190567	0.00000000
C	-6.12637048	1.40188628	0.00000000
C	-7.35168874	-0.72717654	0.00000000
C	-7.35168869	0.72715710	0.00000000
C	-8.57692353	-1.40190655	0.00000000
C	-8.57692328	1.40188722	0.00000000
C	-9.80223210	-0.72716642	0.00000000
C	-9.80223187	0.72714744	0.00000000
C	-11.02749371	-1.40189977	0.00000000
C	-11.02749298	1.40188124	0.00000000
C	-12.25274710	-0.72714719	0.00000000
C	-12.25274659	0.72712949	0.00000000
C	-13.47809587	-1.40187891	0.00000000
C	-13.47809457	1.40186213	0.00000000
C	-14.70322694	-0.72712300	0.00000000

C	-14.70322613	0.72710756	0.00000000
C	-15.92873441	-1.40184461	0.00000000
C	-15.92873258	1.40183055	0.00000000
C	-17.15369699	-0.72711621	0.00000000
C	-17.15369588	0.72710390	0.00000000
C	-18.37938398	-1.40180992	0.00000000
C	-18.37938165	1.40179946	0.00000000
C	-19.60423629	-0.72715961	0.00000000
C	-19.60423496	0.72715129	0.00000000
C	-20.82996311	-1.40180430	0.00000000
C	-20.82996039	1.40179826	0.00000000
C	-22.05498078	-0.72728850	0.00000000
C	-22.05497929	0.72728491	0.00000000
C	-23.28033375	-1.40187967	0.00000000
C	-23.28033077	1.40187868	0.00000000
C	-24.50608174	-0.72750843	0.00000000
C	-24.50608015	0.72751006	0.00000000
C	-25.73035674	-1.40208725	0.00000000
C	-25.73035363	1.40209161	0.00000000
C	-26.95756844	-0.72773355	0.00000000
C	-26.95756679	0.72774063	0.00000000
C	-28.18004054	-1.40242065	0.00000000
C	-28.18003731	1.40243055	0.00000000
C	-29.40913340	-0.72772478	0.00000000
C	-29.40913169	0.72773753	0.00000000
C	-30.62976415	-1.40272307	0.00000000
C	-30.62976076	1.40273878	0.00000000
C	-31.85988761	-0.72706830	0.00000000
C	-31.85988583	0.72708704	0.00000000
C	-33.08049794	-1.40260212	0.00000000
C	-33.08049439	1.40262391	0.00000000
C	-34.30817195	-0.72520407	0.00000000
C	-34.30817009	0.72522904	0.00000000
C	-35.53424016	-1.40111796	0.00000000
C	-35.53423650	1.40114605	0.00000000
C	-36.75181128	-0.72170515	0.00000000
C	-36.75180937	0.72173648	0.00000000
C	-37.99568303	-1.40199880	0.00000000
C	-37.99567928	1.40203338	0.00000000
C	-39.17880497	-0.70808957	0.00000000
C	-39.17880307	0.70812736	0.00000000
H	40.13306904	-1.24961737	0.00000000
H	40.13306644	1.24965156	0.00000000
H	37.98787235	-2.50082067	0.00000000
H	37.98786716	2.50085035	0.00000000
H	35.53525038	-2.50132000	0.00000000
H	35.53524532	2.50134461	0.00000000
H	33.08095942	-2.50268708	0.00000000
H	33.08095444	2.50270679	0.00000000
H	30.62966174	-2.50282255	0.00000000
H	30.62965704	2.50283757	0.00000000
H	28.17972761	-2.50254484	0.00000000
H	28.17972315	2.50255545	0.00000000
H	25.73009326	-2.50223056	0.00000000
H	25.73008892	2.50223687	0.00000000
H	23.28021471	-2.50203362	0.00000000
H	23.28021035	2.50203565	0.00000000
H	20.82996113	-2.50196155	0.00000000
H	20.82995694	2.50195932	0.00000000
H	18.37943393	-2.50196627	0.00000000
H	18.37943018	2.50196008	0.00000000
H	15.92878693	-2.50199856	0.00000000
H	15.92878370	2.50198886	0.00000000
H	13.47812752	-2.50203066	0.00000000
H	13.47812487	2.50201809	0.00000000
H	11.02750317	-2.50205037	0.00000000
H	11.02750133	2.50203564	0.00000000
H	8.57691951	-2.50205683	0.00000000
H	8.57691834	2.50204072	0.00000000
H	6.12636226	-2.50205617	0.00000000
H	6.12636162	2.50203926	0.00000000
H	3.67581624	-2.50205303	0.00000000
H	3.67581578	2.50203563	0.00000000
H	1.22527201	-2.50205101	0.00000000
H	1.22527156	2.50203317	0.00000000
H	-1.22527252	-2.50205126	0.00000000
H	-1.22527322	2.50203287	0.00000000
H	-3.67581650	-2.50205378	0.00000000
H	-3.67581705	2.50203477	0.00000000
H	-6.12636218	-2.50205736	0.00000000
H	-6.12636238	2.50203792	0.00000000
H	-8.57691903	-2.50205843	0.00000000
H	-8.57691856	2.50203900	0.00000000

H	-11.02750245	-2.50205229	0.00000000
H	-11.02750110	2.50203364	0.00000000
H	-13.47812677	-2.50203283	0.00000000
H	-13.47812443	2.50201591	0.00000000
H	-15.92878648	-2.50200084	0.00000000
H	-15.92878326	2.50198665	0.00000000
H	-18.37943398	-2.50196852	0.00000000
H	-18.37942989	2.50195795	0.00000000
H	-20.82996173	-2.50196352	0.00000000
H	-20.82995689	2.50195744	0.00000000
H	-23.28021576	-2.50203516	0.00000000
H	-23.28021044	2.50203416	0.00000000
H	-25.73009452	-2.50223153	0.00000000
H	-25.73008899	2.50223589	0.00000000
H	-28.17972875	-2.50254516	0.00000000
H	-28.17972300	2.50255505	0.00000000
H	-30.62966253	-2.50282216	0.00000000
H	-30.62965642	2.50283784	0.00000000
H	-33.08095977	-2.50268598	0.00000000
H	-33.08095337	2.50270774	0.00000000
H	-35.53525040	-2.50131820	0.00000000
H	-35.53524389	2.50134626	0.00000000
H	-37.98787220	-2.50081816	0.00000000
H	-37.98786554	2.50085271	0.00000000
H	-40.13306844	-1.24961428	0.00000000
H	-40.13306510	1.24965460	0.00000000

32-acene (triplet), E = -4949.5588146693

C	39.17977005	-0.70804795	0.00000000
C	39.17977174	0.70802774	0.00000000
C	37.99651825	-1.40196652	0.00000000
C	37.99652153	1.40194897	0.00000000
C	36.75277846	-0.72167265	0.00000000
C	36.75278011	0.72165774	0.00000000
C	35.53501687	-1.40108908	0.00000000
C	35.53501985	1.40107668	0.00000000
C	34.30906487	-0.72519538	0.00000000
C	34.30906621	0.72518499	0.00000000
C	33.08125644	-1.40257579	0.00000000
C	33.08125874	1.40256733	0.00000000
C	31.86062961	-0.72706802	0.00000000
C	31.86063056	0.72706108	0.00000000
C	30.63052520	-1.40270090	0.00000000
C	30.63052688	1.40269531	0.00000000
C	29.40970995	-0.72770773	0.00000000
C	29.40971069	0.72770347	0.00000000
C	28.18078152	-1.40240523	0.00000000
C	28.18078288	1.40240208	0.00000000
C	26.95803286	-0.72768769	0.00000000
C	26.95803353	0.72768594	0.00000000
C	25.73102859	-1.40208083	0.00000000
C	25.73102984	1.40208023	0.00000000
C	24.50650894	-0.72744277	0.00000000
C	24.50650955	0.72744374	0.00000000
C	23.28090128	-1.40188266	0.00000000
C	23.28090254	1.40188489	0.00000000
C	22.05541574	-0.72722084	0.00000000
C	22.05541633	0.72722474	0.00000000
C	20.83042486	-1.40181374	0.00000000
C	20.83042617	1.40181898	0.00000000
C	19.60467880	-0.72710169	0.00000000
C	19.60467938	0.72710860	0.00000000
C	18.37976187	-1.40182010	0.00000000
C	18.37976312	1.40182837	0.00000000
C	17.15411926	-0.72706928	0.00000000
C	17.15411974	0.72707911	0.00000000
C	15.92905368	-1.40185029	0.00000000
C	15.92905464	1.40186138	0.00000000
C	14.70359853	-0.72708170	0.00000000
C	14.70359881	0.72709398	0.00000000
C	13.47837219	-1.40187720	0.00000000
C	13.47837263	1.40189040	0.00000000
C	12.25304934	-0.72710531	0.00000000
C	12.25304932	0.72711916	0.00000000
C	11.02773098	-1.40189140	0.00000000
C	11.02773081	1.40190575	0.00000000
C	9.80246084	-0.72712058	0.00000000
C	9.80246051	0.72713498	0.00000000
C	8.57711770	-1.40189424	0.00000000
C	8.57711689	1.40190855	0.00000000
C	7.35184930	-0.72712644	0.00000000
C	7.35184866	0.72714025	0.00000000
C	6.12651491	-1.40189253	0.00000000
C	6.12651348	1.40190571	0.00000000

C	4.90123087	-0.72712657	0.00000000
C	4.90122997	0.72713872	0.00000000
C	3.67591199	-1.40189017	0.00000000
C	3.67591003	1.40190116	0.00000000
C	2.45061433	-0.72712556	0.00000000
C	2.45061322	0.72713513	0.00000000
C	1.22530564	-1.40188971	0.00000000
C	1.22530335	1.40189777	0.00000000
C	0.00000100	-0.72712610	0.00000000
C	-0.00000022	0.72713256	0.00000000
C	-1.22530254	-1.40189141	0.00000000
C	-1.22530491	1.40189617	0.00000000
C	-2.45061252	-0.72712881	0.00000000
C	-2.45061369	0.72713199	0.00000000
C	-3.67590937	-1.40189504	0.00000000
C	-3.67591155	1.40189656	0.00000000
C	-4.90122951	-0.72713265	0.00000000
C	-4.90123056	0.72713282	0.00000000
C	-6.12651310	-1.40189989	0.00000000
C	-6.12651490	1.40189869	0.00000000
C	-7.35184855	-0.72713452	0.00000000
C	-7.35184941	0.72713237	0.00000000
C	-8.57711683	-1.40190312	0.00000000
C	-8.57711818	1.40189999	0.00000000
C	-9.80246072	-0.72712968	0.00000000
C	-9.80246136	0.72712603	0.00000000
C	-11.02773098	-1.40190075	0.00000000
C	-11.02773183	1.40189657	0.00000000
C	-12.25304970	-0.72711438	0.00000000
C	-12.25305012	0.72711014	0.00000000
C	-13.47837282	-1.40188595	0.00000000
C	-13.47837323	1.40188162	0.00000000
C	-14.70359911	-0.72708986	0.00000000
C	-14.70359934	0.72708575	0.00000000
C	-15.92905458	-1.40185767	0.00000000
C	-15.92905469	1.40185378	0.00000000
C	-17.15411976	-0.72707590	0.00000000
C	-17.15411987	0.72707233	0.00000000
C	-18.37976264	-1.40182566	0.00000000
C	-18.37976265	1.40182249	0.00000000
C	-19.60467899	-0.72710650	0.00000000
C	-19.60467911	0.72710360	0.00000000
C	-20.83042521	-1.40181742	0.00000000
C	-20.83042530	1.40181497	0.00000000
C	-22.05541549	-0.72722389	0.00000000
C	-22.05541568	0.72722153	0.00000000
C	-23.28090116	-1.40188472	0.00000000
C	-23.28090145	1.40188260	0.00000000
C	-24.50650841	-0.72744433	0.00000000
C	-24.50650866	0.72744211	0.00000000
C	-25.73102822	-1.40208161	0.00000000
C	-25.73102869	1.40207940	0.00000000
C	-26.95803233	-0.72768812	0.00000000
C	-26.95803259	0.72768555	0.00000000
C	-28.18078129	-1.40240516	0.00000000
C	-28.18078182	1.40240229	0.00000000
C	-29.40970974	-0.72770739	0.00000000
C	-29.40970998	0.72770397	0.00000000
C	-30.63052560	-1.40270016	0.00000000
C	-30.63052591	1.40269633	0.00000000
C	-31.86063000	-0.72706677	0.00000000
C	-31.86063008	0.72706254	0.00000000
C	-33.08125787	-1.40257398	0.00000000
C	-33.08125761	1.40256948	0.00000000
C	-34.30906607	-0.72519246	0.00000000
C	-34.30906579	0.72518811	0.00000000
C	-35.53501934	-1.40108515	0.00000000
C	-35.53501847	1.40108096	0.00000000
C	-36.75278028	-0.72166704	0.00000000
C	-36.75277971	0.72166351	0.00000000
C	-37.99652129	-1.40195925	0.00000000
C	-37.99652013	1.40195649	0.00000000
C	-39.17977211	-0.70803884	0.00000000
C	-39.17977150	0.70803697	0.00000000
H	40.13399538	-1.24963688	0.00000000
H	40.13399834	1.24961443	0.00000000
H	37.98871114	-2.50078564	0.00000000
H	37.98871694	2.50076819	0.00000000
H	35.53603132	-2.50128934	0.00000000
H	35.53603659	2.50127713	0.00000000
H	33.08171219	-2.50265963	0.00000000
H	33.08171638	2.50265138	0.00000000
H	30.63041612	-2.50279938	0.00000000

H	30.63041921	2.50279390	0.00000000
H	28.18047380	-2.50252820	0.00000000
H	28.18047625	2.50252506	0.00000000
H	25.73078374	-2.50222263	0.00000000
H	25.73078594	2.50222196	0.00000000
H	23.28080284	-2.50203486	0.00000000
H	23.28080500	2.50203699	0.00000000
H	20.83043348	-2.50196912	0.00000000
H	20.83043565	2.50197427	0.00000000
H	18.37980915	-2.50197466	0.00000000
H	18.37981115	2.50198291	0.00000000
H	15.92909530	-2.50200259	0.00000000
H	15.92909675	2.50201375	0.00000000
H	13.47839238	-2.50202745	0.00000000
H	13.47839293	2.50204080	0.00000000
H	11.02773287	-2.50204050	0.00000000
H	11.02773241	2.50205502	0.00000000
H	8.57711160	-2.50204284	0.00000000
H	8.57711006	2.50205734	0.00000000
H	6.12650882	-2.50204099	0.00000000
H	6.12650627	2.50205433	0.00000000
H	3.67590905	-2.50203876	0.00000000
H	3.67590561	2.50204987	0.00000000
H	1.22530549	-2.50203845	0.00000000
H	1.22530149	2.50204655	0.00000000
H	-1.22530059	-2.50204023	0.00000000
H	-1.22530475	2.50204494	0.00000000
H	-3.67590480	-2.50204385	0.00000000
H	-3.67590865	2.50204524	0.00000000
H	-6.12650571	-2.50204863	0.00000000
H	-6.12650892	2.50204726	0.00000000
H	-8.57710981	-2.50205201	0.00000000
H	-8.57711227	2.50204869	0.00000000
H	-11.02773237	-2.50205008	0.00000000
H	-11.02773401	2.50204573	0.00000000
H	-13.47839285	-2.50203633	0.00000000
H	-13.47839378	2.50203186	0.00000000
H	-15.92909631	-2.50200996	0.00000000
H	-15.92909676	2.50200600	0.00000000
H	-18.37981018	-2.50198008	0.00000000
H	-18.37981045	2.50197694	0.00000000
H	-20.83043412	-2.50197259	0.00000000
H	-20.83043446	2.50197024	0.00000000
H	-23.28080296	-2.50203673	0.00000000
H	-23.28080360	2.50203472	0.00000000
H	-25.73078360	-2.50222333	0.00000000
H	-25.73078449	2.50222120	0.00000000
H	-28.18047387	-2.50252820	0.00000000
H	-28.18047483	2.50252534	0.00000000
H	-30.63041717	-2.50279886	0.00000000
H	-30.63041766	2.50279493	0.00000000
H	-33.08171478	-2.50265816	0.00000000
H	-33.08171425	2.50265346	0.00000000
H	-35.53603532	-2.50128572	0.00000000
H	-35.53603384	2.50128133	0.00000000
H	-37.98871592	-2.50077855	0.00000000
H	-37.98871390	2.50077571	0.00000000
H	-40.13399845	-1.24962631	0.00000000
H	-40.13399740	1.24962521	0.00000000

34-acene (singlet), E = -5254.0444034331

C	41.62930421	-0.70808259	0.00000000
C	41.62930210	0.70813147	0.00000000
C	40.44618135	-1.40199554	0.00000000
C	40.44617720	1.40204096	0.00000000
C	39.20231352	-0.72169980	0.00000000
C	39.20231140	0.72174156	0.00000000
C	37.98474015	-1.40111516	0.00000000
C	37.98473609	1.40115339	0.00000000
C	36.75867497	-0.72519972	0.00000000
C	36.75867290	0.72523446	0.00000000
C	35.53100045	-1.40259962	0.00000000
C	35.53099654	1.40263092	0.00000000
C	34.31039065	-0.72706413	0.00000000
C	34.31038864	0.72709205	0.00000000
C	33.08026864	-1.40272153	0.00000000
C	33.08026479	1.40274609	0.00000000
C	31.85963590	-0.72771996	0.00000000
C	31.85963388	0.72774115	0.00000000
C	30.63054738	-1.40241864	0.00000000
C	30.63054351	1.40243649	0.00000000
C	29.40807375	-0.72772965	0.00000000
C	29.40807172	0.72774412	0.00000000
C	28.18086504	-1.40208583	0.00000000

C	28.18086115	1.40209694	0.00000000
C	26.95658945	-0.72750465	0.00000000
C	26.95658742	0.72751239	0.00000000
C	25.73084439	-1.40187992	0.00000000
C	25.73084058	1.40188433	0.00000000
C	24.50549291	-0.72728534	0.00000000
C	24.50549096	0.72728648	0.00000000
C	23.28047731	-1.40180427	0.00000000
C	23.28047369	1.40180226	0.00000000
C	22.05475282	-0.72715693	0.00000000
C	22.05475101	0.72715185	0.00000000
C	20.82990263	-1.40181068	0.00000000
C	20.82989935	1.40180268	0.00000000
C	19.60421891	-0.72711537	0.00000000
C	19.60421732	0.72710463	0.00000000
C	18.37925779	-1.40184715	0.00000000
C	18.37925502	1.40183388	0.00000000
C	17.15375223	-0.72712299	0.00000000
C	17.15375094	0.72710742	0.00000000
C	15.92862271	-1.40188119	0.00000000
C	15.92862050	1.40186354	0.00000000
C	14.70327549	-0.72714667	0.00000000
C	14.70327447	0.72712720	0.00000000
C	13.47802468	-1.40190250	0.00000000
C	13.47802295	1.40188141	0.00000000
C	12.25276466	-0.72716830	0.00000000
C	12.25276388	0.72714576	0.00000000
C	11.02745875	-1.40191124	0.00000000
C	11.02745741	1.40188745	0.00000000
C	9.80222390	-0.72717917	0.00000000
C	9.80222327	0.72715425	0.00000000
C	8.57691049	-1.40191139	0.00000000
C	8.57690944	1.40188554	0.00000000
C	7.35166879	-0.72718239	0.00000000
C	7.35166830	0.72715564	0.00000000
C	6.12636671	-1.40190893	0.00000000
C	6.12636592	1.40188148	0.00000000
C	4.90111018	-0.72718162	0.00000000
C	4.90110983	0.72715353	0.00000000
C	3.67582132	-1.40190624	0.00000000
C	3.67582082	1.40187770	0.00000000
C	2.45055325	-0.72718008	0.00000000
C	2.45055307	0.72715119	0.00000000
C	1.22527323	-1.40190487	0.00000000
C	1.22527307	1.40187578	0.00000000
C	-0.00000128	-0.72717939	0.00000000
C	-0.00000128	0.72715027	0.00000000
C	-1.22527577	-1.40190482	0.00000000
C	-1.22527560	1.40187576	0.00000000
C	-2.45055547	-0.72717999	0.00000000
C	-2.45055528	0.72715114	0.00000000
C	-3.67582320	-1.40190612	0.00000000
C	-3.67582268	1.40187764	0.00000000
C	-4.90111150	-0.72718146	0.00000000
C	-4.90111115	0.72715346	0.00000000
C	-6.12636745	-1.40190876	0.00000000
C	-6.12636666	1.40188140	0.00000000
C	-7.35166890	-0.72718221	0.00000000
C	-7.35166841	0.72715556	0.00000000
C	-8.57690997	-1.40191123	0.00000000
C	-8.57690892	1.40188546	0.00000000
C	-9.80222284	-0.72717902	0.00000000
C	-9.80222223	0.72715418	0.00000000
C	-11.02745720	-1.40191111	0.00000000
C	-11.02745586	1.40188742	0.00000000
C	-12.25276285	-0.72716822	0.00000000
C	-12.25276205	0.72714573	0.00000000
C	-13.47802262	-1.40190247	0.00000000
C	-13.47802091	1.40188140	0.00000000
C	-14.70327350	-0.72714669	0.00000000
C	-14.70327249	0.72712721	0.00000000
C	-15.92862082	-1.40188123	0.00000000
C	-15.92861862	1.40186359	0.00000000
C	-17.15375071	-0.72712307	0.00000000
C	-17.15374942	0.72710748	0.00000000
C	-18.37925667	-1.40184726	0.00000000
C	-18.37925391	1.40183395	0.00000000
C	-19.60421833	-0.72711550	0.00000000
C	-19.60421677	0.72710472	0.00000000
C	-20.82990262	-1.40181081	0.00000000
C	-20.82989937	1.40180275	0.00000000
C	-22.05475339	-0.72715707	0.00000000
C	-22.05475161	0.72715194	0.00000000

C	-23.28047845	-1.40180438	0.00000000
C	-23.28047484	1.40180232	0.00000000
C	-24.50549445	-0.72728543	0.00000000
C	-24.50549251	0.72728654	0.00000000
C	-25.73084631	-1.40187997	0.00000000
C	-25.73084249	1.40188438	0.00000000
C	-26.95659145	-0.72750466	0.00000000
C	-26.95658945	0.72751241	0.00000000
C	-28.18086713	-1.40208581	0.00000000
C	-28.18086324	1.40209694	0.00000000
C	-29.40807560	-0.72772960	0.00000000
C	-29.40807358	0.72774408	0.00000000
C	-30.63054898	-1.40241856	0.00000000
C	-30.63054512	1.40243645	0.00000000
C	-31.85963701	-0.72771986	0.00000000
C	-31.85963500	0.72774107	0.00000000
C	-33.08026926	-1.40272144	0.00000000
C	-33.08026542	1.40274602	0.00000000
C	-34.31039069	-0.72706402	0.00000000
C	-34.31038869	0.72709193	0.00000000
C	-35.53099994	-1.40259950	0.00000000
C	-35.53099604	1.40263080	0.00000000
C	-36.75867395	-0.72519962	0.00000000
C	-36.75867188	0.72523433	0.00000000
C	-37.98473865	-1.40111508	0.00000000
C	-37.98473459	1.40115328	0.00000000
C	-39.20231164	-0.72169971	0.00000000
C	-39.20230950	0.72174143	0.00000000
C	-40.44617915	-1.40199544	0.00000000
C	-40.44617499	1.40204080	0.00000000
C	-41.62930181	-0.70808252	0.00000000
C	-41.62929970	0.70813136	0.00000000
H	42.58356306	-1.24960690	0.00000000
H	42.58355933	1.24965863	0.00000000
H	40.43837420	-2.50081464	0.00000000
H	40.43836680	2.50086003	0.00000000
H	37.98575283	-2.50131540	0.00000000
H	37.98574559	2.50135361	0.00000000
H	35.53146208	-2.50268370	0.00000000
H	35.53145512	2.50271500	0.00000000
H	33.08016702	-2.50282064	0.00000000
H	33.08016017	2.50284524	0.00000000
H	30.63023759	-2.50254310	0.00000000
H	30.63023074	2.50256102	0.00000000
H	28.18060188	-2.50222990	0.00000000
H	28.18059497	2.50224108	0.00000000
H	25.73072546	-2.50203485	0.00000000
H	25.73071868	2.50203929	0.00000000
H	23.28047636	-2.50196296	0.00000000
H	23.28046992	2.50196092	0.00000000
H	20.82995340	-2.50196867	0.00000000
H	20.82994756	2.50196058	0.00000000
H	18.37930934	-2.50200280	0.00000000
H	18.37930441	2.50198941	0.00000000
H	15.92865480	-2.50203454	0.00000000
H	15.92865086	2.50201678	0.00000000
H	13.47803580	-2.50205423	0.00000000
H	13.47803272	2.50203307	0.00000000
H	11.02745634	-2.50206228	0.00000000
H	11.02745393	2.50203847	0.00000000
H	8.57690341	-2.50206228	0.00000000
H	8.57690154	2.50203643	0.00000000
H	6.12636052	-2.50205984	0.00000000
H	6.12635912	2.50203241	0.00000000
H	3.67581794	-2.50205733	0.00000000
H	3.67581709	2.50202878	0.00000000
H	1.22527216	-2.50205604	0.00000000
H	1.22527191	2.50202694	0.00000000
H	-1.22527504	-2.50205596	0.00000000
H	-1.22527475	2.50202689	0.00000000
H	-3.67582007	-2.50205711	0.00000000
H	-3.67581917	2.50202864	0.00000000
H	-6.12636133	-2.50205956	0.00000000
H	-6.12635993	2.50203221	0.00000000
H	-8.57690277	-2.50206200	0.00000000
H	-8.57690091	2.50203624	0.00000000
H	-11.02745451	-2.50206208	0.00000000
H	-11.02745214	2.50203836	0.00000000
H	-13.47803340	-2.50205418	0.00000000
H	-13.47803037	2.50203303	0.00000000
H	-15.92865261	-2.50203462	0.00000000
H	-15.92864869	2.50201687	0.00000000
H	-18.37930803	-2.50200299	0.00000000

H	-18.37930312	2.50198957	0.00000000
H	-20.82995338	-2.50196890	0.00000000
H	-20.82994759	2.50196077	0.00000000
H	-23.28047768	-2.50196315	0.00000000
H	-23.28047124	2.50196107	0.00000000
H	-25.73072770	-2.50203495	0.00000000
H	-25.73072088	2.50203938	0.00000000
H	-28.18060430	-2.50222987	0.00000000
H	-28.18059739	2.50224106	0.00000000
H	-30.63023943	-2.50254295	0.00000000
H	-30.63023257	2.50256090	0.00000000
H	-33.08016770	-2.50282045	0.00000000
H	-33.08016088	2.50284506	0.00000000
H	-35.53146149	-2.50268348	0.00000000
H	-35.53145454	2.50271477	0.00000000
H	-37.98575119	-2.50131522	0.00000000
H	-37.98574396	2.50135339	0.00000000
H	-40.43837189	-2.50081446	0.00000000
H	-40.43836449	2.50085979	0.00000000
H	-42.58356057	-1.24960690	0.00000000
H	-42.58355684	1.24965858	0.00000000

34-acene (triplet), E = -5254.0420288482

C	41.63021197	-0.70804812	0.00000000
C	41.63021225	0.70804082	0.00000000
C	40.44697590	-1.40196973	0.00000000
C	40.44697648	1.40196292	0.00000000
C	39.20322479	-0.72167452	0.00000000
C	39.20322508	0.72166822	0.00000000
C	37.98548466	-1.40109356	0.00000000
C	37.98548525	1.40108779	0.00000000
C	36.75952233	-0.72519627	0.00000000
C	36.75952263	0.72519101	0.00000000
C	35.53173015	-1.40258078	0.00000000
C	35.53173072	1.40257601	0.00000000
C	34.31110688	-0.72706832	0.00000000
C	34.31110718	0.72706406	0.00000000
C	33.08100258	-1.40270622	0.00000000
C	33.08100316	1.40270248	0.00000000
C	31.86020894	-0.72770925	0.00000000
C	31.86020924	0.72770601	0.00000000
C	30.63126645	-1.40240893	0.00000000
C	30.63126704	1.40240621	0.00000000
C	29.40855063	-0.72769328	0.00000000
C	29.40855093	0.72769107	0.00000000
C	28.18152635	-1.40208377	0.00000000
C	28.18152693	1.40208207	0.00000000
C	26.95703588	-0.72745063	0.00000000
C	26.95703618	0.72744944	0.00000000
C	25.73141607	-1.40188622	0.00000000
C	25.73141664	1.40188553	0.00000000
C	24.50594735	-0.72722966	0.00000000
C	24.50594763	0.72722947	0.00000000
C	23.28095601	-1.40181662	0.00000000
C	23.28095654	1.40181691	0.00000000
C	22.05521316	-0.72711007	0.00000000
C	22.05521342	0.72711083	0.00000000
C	20.83030542	-1.40182409	0.00000000
C	20.83030590	1.40182527	0.00000000
C	19.60465900	-0.72707820	0.00000000
C	19.60465924	0.72707980	0.00000000
C	18.37960520	-1.40185651	0.00000000
C	18.37960562	1.40185848	0.00000000
C	17.15414389	-0.72709062	0.00000000
C	17.15414410	0.72709297	0.00000000
C	15.92892711	-1.40188404	0.00000000
C	15.92892749	1.40188673	0.00000000
C	14.70360107	-0.72711347	0.00000000
C	14.70360125	0.72711651	0.00000000
C	13.47828789	-1.40189890	0.00000000
C	13.47828822	1.40190223	0.00000000
C	12.25301870	-0.72713084	0.00000000
C	12.25301886	0.72713448	0.00000000
C	11.02767589	-1.40190322	0.00000000
C	11.02767616	1.40190710	0.00000000
C	9.80240933	-0.72713684	0.00000000
C	9.80240946	0.72714096	0.00000000
C	8.57707529	-1.40190106	0.00000000
C	8.57707550	1.40190536	0.00000000
C	7.35179208	-0.72713616	0.00000000
C	7.35179217	0.72714066	0.00000000
C	6.12647551	-1.40189772	0.00000000
C	6.12647565	1.40190235	0.00000000
C	4.90117816	-0.72713294	0.00000000

C	4.90117820	0.72713770	0.00000000
C	3.67587391	-1.40189477	0.00000000
C	3.67587398	1.40189959	0.00000000
C	2.45057134	-0.72713014	0.00000000
C	2.45057136	0.72713502	0.00000000
C	1.22527146	-1.40189319	0.00000000
C	1.22527146	1.40189807	0.00000000
C	-0.00002947	-0.72712893	0.00000000
C	-0.00002948	0.72713381	0.00000000
C	-1.22532981	-1.40189271	0.00000000
C	-1.22532985	1.40189753	0.00000000
C	-2.45062811	-0.72712950	0.00000000
C	-2.45062815	0.72713429	0.00000000
C	-3.67592797	-1.40189332	0.00000000
C	-3.67592807	1.40189805	0.00000000
C	-4.90122854	-0.72713168	0.00000000
C	-4.90122860	0.72713631	0.00000000
C	-6.12652127	-1.40189540	0.00000000
C	-6.12652143	1.40189990	0.00000000
C	-7.35183236	-0.72713436	0.00000000
C	-7.35183246	0.72713873	0.00000000
C	-8.57710948	-1.40189808	0.00000000
C	-8.57710969	1.40190226	0.00000000
C	-9.80243683	-0.72713470	0.00000000
C	-9.80243696	0.72713870	0.00000000
C	-11.02769650	-1.40189997	0.00000000
C	-11.02769677	1.40190373	0.00000000
C	-12.25303232	-0.72712864	0.00000000
C	-12.25303248	0.72713216	0.00000000
C	-13.47829466	-1.40189582	0.00000000
C	-13.47829498	1.40189905	0.00000000
C	-14.70360155	-0.72711148	0.00000000
C	-14.70360175	0.72711446	0.00000000
C	-15.92892170	-1.40188154	0.00000000
C	-15.92892208	1.40188420	0.00000000
C	-17.15413364	-0.72708909	0.00000000
C	-17.15413385	0.72709141	0.00000000
C	-18.37959082	-1.40185487	0.00000000
C	-18.37959123	1.40185685	0.00000000
C	-19.60464161	-0.72707718	0.00000000
C	-19.60464183	0.72707879	0.00000000
C	-20.83028576	-1.40182323	0.00000000
C	-20.83028620	1.40182443	0.00000000
C	-22.05519192	-0.72710940	0.00000000
C	-22.05519216	0.72711022	0.00000000
C	-23.28093385	-1.40181624	0.00000000
C	-23.28093435	1.40181662	0.00000000
C	-24.50592428	-0.72722917	0.00000000
C	-24.50592456	0.72722913	0.00000000
C	-25.73139278	-1.40188613	0.00000000
C	-25.73139333	1.40188562	0.00000000
C	-26.95701187	-0.72745035	0.00000000
C	-26.95701217	0.72744936	0.00000000
C	-28.18150262	-1.40208405	0.00000000
C	-28.18150321	1.40208254	0.00000000
C	-29.40852667	-0.72769335	0.00000000
C	-29.40852698	0.72769130	0.00000000
C	-30.63124333	-1.40240956	0.00000000
C	-30.63124392	1.40240700	0.00000000
C	-31.86018643	-0.72770956	0.00000000
C	-31.86018674	0.72770647	0.00000000
C	-33.08098108	-1.40270690	0.00000000
C	-33.08098171	1.40270323	0.00000000
C	-34.31108634	-0.72706856	0.00000000
C	-34.31108667	0.72706433	0.00000000
C	-35.53171005	-1.40258120	0.00000000
C	-35.53171069	1.40257642	0.00000000
C	-36.75950280	-0.72519632	0.00000000
C	-36.75950313	0.72519100	0.00000000
C	-37.98546499	-1.40109411	0.00000000
C	-37.98546567	1.40108819	0.00000000
C	-39.20320567	-0.72167495	0.00000000
C	-39.20320602	0.72166845	0.00000000
C	-40.44695724	-1.40197073	0.00000000
C	-40.44695791	1.40196364	0.00000000
C	-41.63019425	-0.70804882	0.00000000
C	-41.63019459	0.70804117	0.00000000
H	42.58443729	-1.24962849	0.00000000
H	42.58443780	1.24962080	0.00000000
H	40.43917239	-2.50078834	0.00000000
H	40.43917341	2.50078154	0.00000000
H	37.98650151	-2.50129349	0.00000000
H	37.98650257	2.50128772	0.00000000

H	35.53218686	-2.50266444	0.00000000
H	35.53218788	2.50265968	0.00000000
H	33.08089447	-2.50280430	0.00000000
H	33.08089550	2.50280056	0.00000000
H	30.63096064	-2.50253144	0.00000000
H	30.63096169	2.50252872	0.00000000
H	28.18127863	-2.50222508	0.00000000
H	28.18127966	2.50222336	0.00000000
H	25.73131439	-2.50203786	0.00000000
H	25.73131541	2.50203717	0.00000000
H	23.28096385	-2.50197189	0.00000000
H	23.28096482	2.50197218	0.00000000
H	20.83035371	-2.50197893	0.00000000
H	20.83035456	2.50198010	0.00000000
H	18.37964698	-2.50200957	0.00000000
H	18.37964773	2.50201154	0.00000000
H	15.92894837	-2.50203550	0.00000000
H	15.92894906	2.50203819	0.00000000
H	13.47829173	-2.50204940	0.00000000
H	13.47829232	2.50205274	0.00000000
H	11.02767038	-2.50205347	0.00000000
H	11.02767086	2.50205736	0.00000000
H	8.57706870	-2.50205125	0.00000000
H	8.57706907	2.50205555	0.00000000
H	6.12647167	-2.50204762	0.00000000
H	6.12647192	2.50205225	0.00000000
H	3.67587288	-2.50204425	0.00000000
H	3.67587300	2.50204907	0.00000000
H	1.22527141	-2.50204214	0.00000000
H	1.22527141	2.50204702	0.00000000
H	-1.22532974	-2.50204111	0.00000000
H	-1.22532982	2.50204594	0.00000000
H	-3.67592679	-2.50204124	0.00000000
H	-3.67592696	2.50204597	0.00000000
H	-6.12651724	-2.50204285	0.00000000
H	-6.12651752	2.50204735	0.00000000
H	-8.57710274	-2.50204520	0.00000000
H	-8.57710312	2.50204938	0.00000000
H	-11.02769102	-2.50204689	0.00000000
H	-11.02769150	2.50205065	0.00000000
H	-13.47829880	-2.50204317	0.00000000
H	-13.47829936	2.50204640	0.00000000
H	-15.92894354	-2.50203042	0.00000000
H	-15.92894421	2.50203308	0.00000000
H	-18.37963325	-2.50200619	0.00000000
H	-18.37963399	2.50200817	0.00000000
H	-20.83033450	-2.50197713	0.00000000
H	-20.83033530	2.50197834	0.00000000
H	-23.28094185	-2.50197116	0.00000000
H	-23.28094274	2.50197155	0.00000000
H	-25.73129124	-2.50203777	0.00000000
H	-25.73129221	2.50203726	0.00000000
H	-28.18125527	-2.50222561	0.00000000
H	-28.18125633	2.50222411	0.00000000
H	-30.63093780	-2.50253261	0.00000000
H	-30.63093887	2.50253005	0.00000000
H	-33.08087262	-2.50280567	0.00000000
H	-33.08087376	2.50280200	0.00000000
H	-35.53216601	-2.50266550	0.00000000
H	-35.53216714	2.50266071	0.00000000
H	-37.98648154	-2.50129448	0.00000000
H	-37.98648274	2.50128856	0.00000000
H	-40.43915402	-2.50078964	0.00000000
H	-40.43915521	2.50078255	0.00000000
H	-42.58442009	-1.24962919	0.00000000
H	-42.58442069	1.24962109	0.00000000

36-acene (singlet), E = -5558.5274621599

C	44.07974834	-0.70815586	0.00000000
C	44.07975123	0.70808180	0.00000000
C	42.89663566	-1.40206523	0.00000000
C	42.89664134	1.40199590	0.00000000
C	41.65276267	-0.72174964	0.00000000
C	41.65276560	0.72168531	0.00000000
C	40.43520681	-1.40116534	0.00000000
C	40.43521246	1.40110589	0.00000000
C	39.20913361	-0.72524383	0.00000000
C	39.20913651	0.72518931	0.00000000
C	37.98147510	-1.40264028	0.00000000
C	37.98148068	1.40259062	0.00000000
C	36.76085930	-0.72709825	0.00000000
C	36.76086217	0.72705353	0.00000000
C	35.53075234	-1.40275401	0.00000000
C	35.53075787	1.40271401	0.00000000

C	34.31011597	-0.72774568	0.00000000
C	34.31011885	0.72771065	0.00000000
C	33.08103981	-1.40244481	0.00000000
C	33.08104534	1.40241444	0.00000000
C	31.85856500	-0.72774621	0.00000000
C	31.85856790	0.72772076	0.00000000
C	30.63136781	-1.40210301	0.00000000
C	30.63137331	1.40208226	0.00000000
C	29.40709324	-0.72751435	0.00000000
C	29.40709609	0.72749843	0.00000000
C	28.18134947	-1.40188911	0.00000000
C	28.18135484	1.40187781	0.00000000
C	26.95600553	-0.72728685	0.00000000
C	26.95600828	0.72728026	0.00000000
C	25.73098932	-1.40180635	0.00000000
C	25.73099452	1.40180426	0.00000000
C	24.50527288	-0.72715147	0.00000000
C	24.50527550	0.72715397	0.00000000
C	23.28042033	-1.40180391	0.00000000
C	23.28042524	1.40181062	0.00000000
C	22.05474360	-0.72710345	0.00000000
C	22.05474604	0.72711449	0.00000000
C	20.82978089	-1.40183468	0.00000000
C	20.82978541	1.40184964	0.00000000
C	19.60428236	-0.72710582	0.00000000
C	19.60428455	0.72712475	0.00000000
C	18.37915151	-1.40186271	0.00000000
C	18.37915549	1.40188512	0.00000000
C	17.15381126	-0.72712392	0.00000000
C	17.15381314	0.72714983	0.00000000
C	15.92855700	-1.40187791	0.00000000
C	15.92856033	1.40190673	0.00000000
C	14.70329901	-0.72713922	0.00000000
C	14.70330056	0.72717102	0.00000000
C	13.47800162	-1.40188302	0.00000000
C	13.47800431	1.40191711	0.00000000
C	12.25276624	-0.72714930	0.00000000
C	12.25276751	0.72718582	0.00000000
C	11.02745396	-1.40188325	0.00000000
C	11.02745612	1.40192155	0.00000000
C	9.80221278	-0.72715004	0.00000000
C	9.80221380	0.72719033	0.00000000
C	8.57691184	-1.40187860	0.00000000
C	8.57691352	1.40192024	0.00000000
C	7.35165666	-0.72714707	0.00000000
C	7.35165647	0.72719023	0.00000000
C	6.12636917	-1.40187526	0.00000000
C	6.12637043	1.40191948	0.00000000
C	4.90110107	-0.72714399	0.00000000
C	4.90110163	0.72718931	0.00000000
C	3.67582312	-1.40187244	0.00000000
C	3.67582391	1.40191849	0.00000000
C	2.45054927	-0.72714182	0.00000000
C	2.45054956	0.72718849	0.00000000
C	1.22527432	-1.40187112	0.00000000
C	1.22527456	1.40191811	0.00000000
C	-0.00000056	-0.72714116	0.00000000
C	-0.00000058	0.72718823	0.00000000
C	-1.22527540	-1.40187113	0.00000000
C	-1.22527571	1.40191803	0.00000000
C	-2.45055030	-0.72714183	0.00000000
C	-2.45055063	0.72718839	0.00000000
C	-3.67582406	-1.40187240	0.00000000
C	-3.67582491	1.40191831	0.00000000
C	-4.90110191	-0.72714400	0.00000000
C	-4.90110252	0.72718916	0.00000000
C	-6.12636989	-1.40187522	0.00000000
C	-6.12637120	1.40191924	0.00000000
C	-7.35165626	-0.72714709	0.00000000
C	-7.35165709	0.72719003	0.00000000
C	-8.57691229	-1.40187859	0.00000000
C	-8.57691403	1.40191994	0.00000000
C	-9.80221311	-0.72715014	0.00000000
C	-9.80221415	0.72719007	0.00000000
C	-11.02745417	-1.40188334	0.00000000
C	-11.02745636	1.40192124	0.00000000
C	-12.25276637	-0.72714947	0.00000000
C	-12.25276764	0.72718554	0.00000000
C	-13.47800165	-1.40188321	0.00000000
C	-13.47800437	1.40191681	0.00000000
C	-14.70329899	-0.72713947	0.00000000
C	-14.70330055	0.72717075	0.00000000
C	-15.92855697	-1.40187815	0.00000000

C	-15.92856029	1.40190651	0.00000000
C	-17.15381121	-0.72712416	0.00000000
C	-17.15381309	0.72714962	0.00000000
C	-18.37915147	-1.40186298	0.00000000
C	-18.37915542	1.40188499	0.00000000
C	-19.60428233	-0.72710604	0.00000000
C	-19.60428452	0.72712461	0.00000000
C	-20.82978089	-1.40183495	0.00000000
C	-20.82978538	1.40184958	0.00000000
C	-22.05474362	-0.72710365	0.00000000
C	-22.05474605	0.72711439	0.00000000
C	-23.28042038	-1.40180416	0.00000000
C	-23.28042526	1.40181057	0.00000000
C	-24.50527294	-0.72715165	0.00000000
C	-24.50527554	0.72715386	0.00000000
C	-25.73098941	-1.40180653	0.00000000
C	-25.73099453	1.40180422	0.00000000
C	-26.95600559	-0.72728692	0.00000000
C	-26.95600830	0.72728022	0.00000000
C	-28.18134951	-1.40188917	0.00000000
C	-28.18135483	1.40187779	0.00000000
C	-29.40709323	-0.72751436	0.00000000
C	-29.40709604	0.72749839	0.00000000
C	-30.63136776	-1.40210298	0.00000000
C	-30.63137320	1.40208222	0.00000000
C	-31.85856486	-0.72774615	0.00000000
C	-31.85856773	0.72772074	0.00000000
C	-33.08103959	-1.40244470	0.00000000
C	-33.08104508	1.40241437	0.00000000
C	-34.31011563	-0.72774559	0.00000000
C	-34.31011850	0.72771062	0.00000000
C	-35.53075194	-1.40275384	0.00000000
C	-35.53075741	1.40271394	0.00000000
C	-36.76085879	-0.72709811	0.00000000
C	-36.76086161	0.72705354	0.00000000
C	-37.98147452	-1.40264007	0.00000000
C	-37.98148003	1.40259060	0.00000000
C	-39.20913291	-0.72524363	0.00000000
C	-39.20913578	0.72518939	0.00000000
C	-40.43520606	-1.40116507	0.00000000
C	-40.43521167	1.40110594	0.00000000
C	-41.65276184	-0.72174943	0.00000000
C	-41.65276476	0.72168544	0.00000000
C	-42.89663480	-1.40206498	0.00000000
C	-42.89664044	1.40199600	0.00000000
C	-44.07974744	-0.70815565	0.00000000
C	-44.07975030	0.70808196	0.00000000
H	45.03403309	-1.24963008	0.00000000
H	45.03403821	1.24955211	0.00000000
H	42.88877714	-2.50088119	0.00000000
H	42.88878725	2.50081188	0.00000000
H	40.43620568	-2.50136306	0.00000000
H	40.43621577	2.50130362	0.00000000
H	37.98191921	-2.50272164	0.00000000
H	37.98192926	2.50267194	0.00000000
H	35.53063397	-2.50285040	0.00000000
H	35.53064385	2.50281031	0.00000000
H	33.08071832	-2.50256615	0.00000000
H	33.08072808	2.50253566	0.00000000
H	30.63110245	-2.50224376	0.00000000
H	30.63111216	2.50222289	0.00000000
H	28.18122463	-2.50204098	0.00000000
H	28.18123418	2.50202959	0.00000000
H	25.73098727	-2.50196219	0.00000000
H	25.73099659	2.50196001	0.00000000
H	23.28047328	-2.50195936	0.00000000
H	23.28048205	2.50196603	0.00000000
H	20.82983285	-2.50198785	0.00000000
H	20.82984095	2.50200280	0.00000000
H	18.37917930	-2.50201443	0.00000000
H	18.37918646	2.50203687	0.00000000
H	15.92856550	-2.50202749	0.00000000
H	15.92857151	2.50205635	0.00000000
H	13.47800652	-2.50203229	0.00000000
H	13.47801132	2.50206639	0.00000000
H	11.02744838	-2.50203193	0.00000000
H	11.02745218	2.50207019	0.00000000
H	8.57690431	-2.50202750	0.00000000
H	8.57690720	2.50206909	0.00000000
H	6.12636585	-2.50202423	0.00000000
H	6.12636799	2.50206838	0.00000000
H	3.67582299	-2.50202157	0.00000000
H	3.67582432	2.50206758	0.00000000

H	1.22527480	-2.50202036	0.00000000
H	1.22527520	2.50206732	0.00000000
H	-1.22527586	-2.50202033	0.00000000
H	-1.22527638	2.50206722	0.00000000
H	-3.67582394	-2.50202146	0.00000000
H	-3.67582534	2.50206733	0.00000000
H	-6.12636657	-2.50202408	0.00000000
H	-6.12636879	2.50206805	0.00000000
H	-8.57690474	-2.50202739	0.00000000
H	-8.57690775	2.50206868	0.00000000
H	-11.02744856	-2.50203193	0.00000000
H	-11.02745244	2.50206980	0.00000000
H	-13.47800652	-2.50203244	0.00000000
H	-13.47801138	2.50206605	0.00000000
H	-15.92856549	-2.50202774	0.00000000
H	-15.92857144	2.50205613	0.00000000
H	-18.37917928	-2.50201474	0.00000000
H	-18.37918637	2.50203678	0.00000000
H	-20.82983286	-2.50198818	0.00000000
H	-20.82984091	2.50200280	0.00000000
H	-23.28047332	-2.50195968	0.00000000
H	-23.28048208	2.50196604	0.00000000
H	-25.73098741	-2.50196241	0.00000000
H	-25.73099655	2.50196002	0.00000000
H	-28.18122468	-2.50204104	0.00000000
H	-28.18123416	2.50202957	0.00000000
H	-30.63110240	-2.50224369	0.00000000
H	-30.63111202	2.50222282	0.00000000
H	-33.08071807	-2.50256597	0.00000000
H	-33.08072779	2.50253553	0.00000000
H	-35.53063353	-2.50285013	0.00000000
H	-35.53064333	2.50281015	0.00000000
H	-37.98191861	-2.50272134	0.00000000
H	-37.98192853	2.50267183	0.00000000
H	-40.43620490	-2.50136272	0.00000000
H	-40.43621493	2.50130358	0.00000000
H	-42.88877627	-2.50088087	0.00000000
H	-42.88878633	2.50081193	0.00000000
H	-45.03403214	-1.24962983	0.00000000
H	-45.03403721	1.24955226	0.00000000

36-acene (triplet), E = -5558.5252247642

C	44.08058477	-0.70802932	0.00000000
C	44.08057912	0.70809823	0.00000000
C	42.89737636	-1.40195541	0.00000000
C	42.89736527	1.40201474	0.00000000
C	41.65360160	-0.72164892	0.00000000
C	41.65359578	0.72169821	0.00000000
C	40.43590153	-1.40107687	0.00000000
C	40.43589110	1.40111610	0.00000000
C	39.20991487	-0.72518035	0.00000000
C	39.20990955	0.72521057	0.00000000
C	37.98215611	-1.40257187	0.00000000
C	37.98214697	1.40259254	0.00000000
C	36.76152374	-0.72705860	0.00000000
C	36.76151918	0.72707139	0.00000000
C	35.53143659	-1.40270515	0.00000000
C	35.53142873	1.40270990	0.00000000
C	34.31065199	-0.72770853	0.00000000
C	34.31064813	0.72770703	0.00000000
C	33.08170858	-1.40241606	0.00000000
C	33.08170205	1.40240824	0.00000000
C	31.85901244	-0.72770005	0.00000000
C	31.85900952	0.72768803	0.00000000
C	30.63198109	-1.40209427	0.00000000
C	30.63197611	1.40207758	0.00000000
C	29.40750940	-0.72746422	0.00000000
C	29.40750753	0.72744520	0.00000000
C	28.18187888	-1.40189866	0.00000000
C	28.18187544	1.40187669	0.00000000
C	26.95642545	-0.72724512	0.00000000
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H	-8.57692311	-2.50207909	0.00000000
H	-8.57691972	2.50202018	0.00000000
H	-11.02746497	-2.50207962	0.00000000
H	-11.02746054	2.50202455	0.00000000
H	-13.47800664	-2.50207999	0.00000000
H	-13.47800102	2.50202976	0.00000000
H	-15.92855811	-2.50207743	0.00000000
H	-15.92855090	2.50203339	0.00000000
H	-18.37913515	-2.50206712	0.00000000
H	-18.37912633	2.50203090	0.00000000
H	-20.82975222	-2.50204409	0.00000000
H	-20.82974199	2.50201721	0.00000000
H	-23.28040504	-2.50200790	0.00000000
H	-23.28039377	2.50199160	0.00000000
H	-25.73104523	-2.50197018	0.00000000
H	-25.73103337	2.50196524	0.00000000
H	-28.18156265	-2.50196140	0.00000000
H	-28.18155051	2.50196818	0.00000000
H	-30.63180492	-2.50202983	0.00000000
H	-30.63179273	2.50204848	0.00000000
H	-33.08167189	-2.50222247	0.00000000
H	-33.08165973	2.50225309	0.00000000
H	-35.53129457	-2.50253341	0.00000000
H	-35.53128247	2.50257597	0.00000000
H	-37.98121911	-2.50280831	0.00000000
H	-37.98120695	2.50286270	0.00000000
H	-40.43252025	-2.50266793	0.00000000
H	-40.43250785	2.50273415	0.00000000
H	-42.88681043	-2.50129509	0.00000000
H	-42.88679786	2.50137340	0.00000000
H	-45.33945905	-2.50078512	0.00000000
H	-45.33944627	2.50087581	0.00000000
H	-47.48457487	-1.24963060	0.00000000
H	-47.48456841	1.24973236	0.00000000

38-acene (triplet), E = -5863.0084054731

C	46.53112336	-0.70805494	0.00000000
C	46.53112392	0.70803614	0.00000000
C	45.34789449	-1.40198023	0.00000000
C	45.34789559	1.40196245	0.00000000
C	44.10413660	-0.72169246	0.00000000
C	44.10413717	0.72167596	0.00000000
C	42.88641843	-1.40110828	0.00000000
C	42.88641963	1.40109305	0.00000000
C	41.66045290	-0.72520741	0.00000000
C	41.66045360	0.72519377	0.00000000
C	40.43267352	-1.40259525	0.00000000
C	40.43267485	1.40258308	0.00000000
C	39.21206790	-0.72707813	0.00000000
C	39.21206868	0.72706756	0.00000000
C	37.98195043	-1.40271996	0.00000000
C	37.98195174	1.40271085	0.00000000
C	36.76120042	-0.72772076	0.00000000
C	36.76120112	0.72771286	0.00000000
C	35.53222252	-1.40242068	0.00000000
C	35.53222359	1.40241387	0.00000000
C	34.30955999	-0.72770774	0.00000000
C	34.30956050	0.72770162	0.00000000
C	33.08249836	-1.40209279	0.00000000
C	33.08249912	1.40208713	0.00000000
C	31.85805017	-0.72746772	0.00000000
C	31.85805057	0.72746229	0.00000000
C	30.63240767	-1.40189257	0.00000000
C	30.63240816	1.40188718	0.00000000
C	29.40695867	-0.72724609	0.00000000
C	29.40695898	0.72724060	0.00000000
C	28.18196623	-1.40182185	0.00000000
C	28.18196661	1.40181617	0.00000000
C	26.95622405	-0.72712394	0.00000000
C	26.95622433	0.72711818	0.00000000
C	25.73133144	-1.40182822	0.00000000
C	25.73133195	1.40182227	0.00000000
C	24.50567691	-0.72708916	0.00000000
C	24.50567731	0.72708348	0.00000000
C	23.28064519	-1.40186055	0.00000000
C	23.28064614	1.40185489	0.00000000
C	22.05517772	-0.72710022	0.00000000
C	22.05517841	0.72709549	0.00000000
C	20.82998219	-1.40188863	0.00000000
C	20.82998370	1.40188430	0.00000000
C	19.60465664	-0.72712229	0.00000000
C	19.60465764	0.72711944	0.00000000
C	18.37936032	-1.40190268	0.00000000
C	18.37936227	1.40190071	0.00000000
C	17.15409895	-0.72713787	0.00000000
C	17.15410016	0.72713762	0.00000000
C	15.92876887	-1.40190492	0.00000000
C	15.92877099	1.40190600	0.00000000
C	14.70351615	-0.72714349	0.00000000
C	14.70351734	0.72714621	0.00000000
C	13.47819136	-1.40190141	0.00000000
C	13.47819327	1.40190560	0.00000000
C	12.25292400	-0.72714251	0.00000000
C	12.25292499	0.72714798	0.00000000
C	11.02761617	-1.40189710	0.00000000
C	11.02761767	1.40190387	0.00000000
C	9.80233267	-0.72713925	0.00000000
C	9.80233339	0.72714687	0.00000000
C	8.57703847	-1.40189433	0.00000000
C	8.57703948	1.40190278	0.00000000
C	7.35174559	-0.72713651	0.00000000
C	7.35174607	0.72714534	0.00000000
C	6.12645776	-1.40189343	0.00000000
C	6.12645837	1.40190258	0.00000000
C	4.90116221	-0.72713516	0.00000000
C	4.90116252	0.72714434	0.00000000
C	3.67587521	-1.40189366	0.00000000
C	3.67587557	1.40190281	0.00000000
C	2.45058084	-0.72713486	0.00000000
C	2.45058107	0.72714383	0.00000000
C	1.22529196	-1.40189423	0.00000000
C	1.22529212	1.40190284	0.00000000
C	0.00000019	-0.72713517	0.00000000
C	0.00000035	0.72714336	0.00000000
C	-1.22529153	-1.40189464	0.00000000
C	-1.22529146	1.40190238	0.00000000
C	-2.45058057	-0.72713568	0.00000000
C	-2.45058044	0.72714297	0.00000000

C	-3.67587505	-1.40189474	0.00000000
C	-3.67587498	1.40190157	0.00000000
C	-4.90116220	-0.72713647	0.00000000
C	-4.90116207	0.72714297	0.00000000
C	-6.12645806	-1.40189480	0.00000000
C	-6.12645789	1.40190097	0.00000000
C	-7.35174599	-0.72713784	0.00000000
C	-7.35174579	0.72714394	0.00000000
C	-8.57703938	-1.40189545	0.00000000
C	-8.57703899	1.40190140	0.00000000
C	-9.80233352	-0.72713991	0.00000000
C	-9.80233317	0.72714611	0.00000000
C	-11.02761769	-1.40189718	0.00000000
C	-11.02761697	1.40190356	0.00000000
C	-12.25292521	-0.72714173	0.00000000
C	-12.25292467	0.72714868	0.00000000
C	-13.47819324	-1.40189972	0.00000000
C	-13.47819229	1.40190715	0.00000000
C	-14.70351745	-0.72714081	0.00000000
C	-14.70351680	0.72714883	0.00000000
C	-15.92877075	-1.40190109	0.00000000
C	-15.92876977	1.40190979	0.00000000
C	-17.15410003	-0.72713323	0.00000000
C	-17.15409946	0.72714223	0.00000000
C	-18.37936169	-1.40189693	0.00000000
C	-18.37936107	1.40190653	0.00000000
C	-19.60465721	-0.72711624	0.00000000
C	-19.60465696	0.72712551	0.00000000
C	-20.82998272	-1.40188185	0.00000000
C	-20.82998280	1.40189125	0.00000000
C	-22.05517768	-0.72709371	0.00000000
C	-22.05517788	0.72710207	0.00000000
C	-23.28064482	-1.40185398	0.00000000
C	-23.28064569	1.40186169	0.00000000
C	-24.50567634	-0.72708331	0.00000000
C	-24.50567695	0.72708941	0.00000000
C	-25.73133039	-1.40182306	0.00000000
C	-25.73133194	1.40182765	0.00000000
C	-26.95622322	-0.72711981	0.00000000
C	-26.95622408	0.72712239	0.00000000
C	-28.18196491	-1.40181887	0.00000000
C	-28.18196686	1.40181931	0.00000000
C	-29.40695786	-0.72724427	0.00000000
C	-29.40695881	0.72724247	0.00000000
C	-30.63240643	-1.40189198	0.00000000
C	-30.63240849	1.40188786	0.00000000
C	-31.85804950	-0.72746819	0.00000000
C	-31.85805047	0.72746186	0.00000000
C	-33.08249740	-1.40209421	0.00000000
C	-33.08249940	1.40208572	0.00000000
C	-34.30955947	-0.72770989	0.00000000
C	-34.30956043	0.72769947	0.00000000
C	-35.53222185	-1.40242338	0.00000000
C	-35.53222373	1.40241110	0.00000000
C	-36.76120005	-0.72772370	0.00000000
C	-36.76120094	0.72770987	0.00000000
C	-37.98194993	-1.40272301	0.00000000
C	-37.98195173	1.40270767	0.00000000
C	-39.21206757	-0.72708114	0.00000000
C	-39.21206844	0.72706449	0.00000000
C	-40.43267295	-1.40259802	0.00000000
C	-40.43267484	1.40258018	0.00000000
C	-41.66045244	-0.72521016	0.00000000
C	-41.66045344	0.72519094	0.00000000
C	-42.88641764	-1.40111083	0.00000000
C	-42.88641973	1.40109037	0.00000000
C	-44.10413600	-0.72169524	0.00000000
C	-44.10413711	0.72167314	0.00000000
C	-45.34789359	-1.40198319	0.00000000
C	-45.34789580	1.40195942	0.00000000
C	-46.53112275	-0.70805826	0.00000000
C	-46.53112387	0.70803276	0.00000000
H	47.48532890	-1.24968689	0.00000000
H	47.48533000	1.24966722	0.00000000
H	45.34015146	-2.50079901	0.00000000
H	45.34015345	2.50078120	0.00000000
H	42.88746066	-2.50130888	0.00000000
H	42.88746282	2.50129359	0.00000000
H	40.43314759	-2.50268003	0.00000000
H	40.43314986	2.50266784	0.00000000
H	37.98184335	-2.50281924	0.00000000
H	37.98184562	2.50281019	0.00000000
H	35.53190882	-2.50254467	0.00000000

H	35.53191084	2.50253796	0.00000000
H	33.08224268	-2.50223591	0.00000000
H	33.08224415	2.50223036	0.00000000
H	30.63229875	-2.50204624	0.00000000
H	30.63229976	2.50204090	0.00000000
H	28.18196925	-2.50197888	0.00000000
H	28.18197016	2.50197316	0.00000000
H	25.73137812	-2.50198436	0.00000000
H	25.73137940	2.50197823	0.00000000
H	23.28068725	-2.50201422	0.00000000
H	23.28068930	2.50200827	0.00000000
H	20.83000267	-2.50203989	0.00000000
H	20.83000548	2.50203525	0.00000000
H	18.37936266	-2.50205226	0.00000000
H	18.37936602	2.50205007	0.00000000
H	15.92876283	-2.50205359	0.00000000
H	15.92876640	2.50205459	0.00000000
H	13.47818459	-2.50204967	0.00000000
H	13.47818788	2.50205393	0.00000000
H	11.02761192	-2.50204523	0.00000000
H	11.02761464	2.50205215	0.00000000
H	8.57703688	-2.50204245	0.00000000
H	8.57703882	2.50205106	0.00000000
H	6.12645769	-2.50204158	0.00000000
H	6.12645897	2.50205085	0.00000000
H	3.67587555	-2.50204183	0.00000000
H	3.67587647	2.50205106	0.00000000
H	1.22529213	-2.50204241	0.00000000
H	1.22529258	2.50205106	0.00000000
H	-1.22529179	-2.50204283	0.00000000
H	-1.22529150	2.50205055	0.00000000
H	-3.67587568	-2.50204292	0.00000000
H	-3.67587536	2.50204971	0.00000000
H	-6.12645847	-2.50204299	0.00000000
H	-6.12645796	2.50204905	0.00000000
H	-8.57703853	-2.50204364	0.00000000
H	-8.57703772	2.50204945	0.00000000
H	-11.02761448	-2.50204537	0.00000000
H	-11.02761317	2.50205162	0.00000000
H	-13.47818762	-2.50204799	0.00000000
H	-13.47818606	2.50205537	0.00000000
H	-15.92876582	-2.50204965	0.00000000
H	-15.92876430	2.50205845	0.00000000
H	-18.37936497	-2.50204629	0.00000000
H	-18.37936400	2.50205615	0.00000000
H	-20.83000386	-2.50203283	0.00000000
H	-20.83000388	2.50204257	0.00000000
H	-23.28068718	-2.50200741	0.00000000
H	-23.28068840	2.50201544	0.00000000
H	-25.73137694	-2.50197908	0.00000000
H	-25.73137933	2.50198388	0.00000000
H	-28.18196747	-2.50197590	0.00000000
H	-28.18197073	2.50197642	0.00000000
H	-30.63229698	-2.50204572	0.00000000
H	-30.63230054	2.50204159	0.00000000
H	-33.08224136	-2.50223743	0.00000000
H	-33.08224478	2.50222886	0.00000000
H	-35.53190796	-2.50254744	0.00000000
H	-35.53191122	2.50253507	0.00000000
H	-37.98184260	-2.50282229	0.00000000
H	-37.98184591	2.50280691	0.00000000
H	-40.43314671	-2.50268271	0.00000000
H	-40.43315020	2.50266491	0.00000000
H	-42.88745953	-2.50131132	0.00000000
H	-42.88746325	2.50129093	0.00000000
H	-45.34015019	-2.50080189	0.00000000
H	-45.34015409	2.50077818	0.00000000
H	-47.48532801	-1.24969042	0.00000000
H	-47.48532994	1.24966357	0.00000000

40-acene (singlet), E = -6167.4935790521

C	48.98081892	-0.70802082	0.00000000
C	48.98081211	0.70818392	0.00000000
C	47.79770012	-1.40195564	0.00000000
C	47.79768668	1.40210738	0.00000000
C	46.55385201	-0.72163626	0.00000000
C	46.55384509	0.72177616	0.00000000
C	45.33626992	-1.40107598	0.00000000
C	45.33625669	1.40120425	0.00000000
C	44.11023843	-0.72516037	0.00000000
C	44.11023165	0.72527726	0.00000000
C	42.88254949	-1.40255616	0.00000000
C	42.88253662	1.40266158	0.00000000
C	41.66195794	-0.72703381	0.00000000

C	41.66195140	0.72712820	0.00000000
C	40.43182894	-1.40269276	0.00000000
C	40.43181659	1.40277615	0.00000000
C	39.21120798	-0.72769691	0.00000000
C	39.21120168	0.72776971	0.00000000
C	37.98212263	-1.40240062	0.00000000
C	37.98211076	1.40246289	0.00000000
C	36.75965297	-0.72771191	0.00000000
C	36.75964691	0.72776402	0.00000000
C	35.53245445	-1.40207454	0.00000000
C	35.53244305	1.40211655	0.00000000
C	34.30817790	-0.72749221	0.00000000
C	34.30817212	0.72752446	0.00000000
C	33.08244412	-1.40187435	0.00000000
C	33.08243331	1.40189699	0.00000000
C	31.85708999	-0.72727854	0.00000000
C	31.85708460	0.72729197	0.00000000
C	30.63208440	-1.40180544	0.00000000
C	30.63207442	1.40180991	0.00000000
C	29.40635839	-0.72715579	0.00000000
C	29.40635348	0.72715181	0.00000000
C	28.18151560	-1.40181719	0.00000000
C	28.18150659	1.40180505	0.00000000
C	26.95583160	-0.72711929	0.00000000
C	26.95582722	0.72709954	0.00000000
C	25.73087592	-1.40185875	0.00000000
C	25.73086793	1.40183175	0.00000000
C	24.50537153	-0.72713243	0.00000000
C	24.50536765	0.72709859	0.00000000
C	23.28024615	-1.40189829	0.00000000
C	23.28023910	1.40185809	0.00000000
C	22.05490020	-0.72716104	0.00000000
C	22.05489677	0.72711477	0.00000000
C	20.82965257	-1.40192370	0.00000000
C	20.82964640	1.40187191	0.00000000
C	19.60439343	-0.72718576	0.00000000
C	19.60439042	0.72712864	0.00000000
C	18.37909045	-1.40193559	0.00000000
C	18.37908510	1.40187372	0.00000000
C	17.15385673	-0.72720069	0.00000000
C	17.15385409	0.72713424	0.00000000
C	15.92854547	-1.40193936	0.00000000
C	15.92854084	1.40186875	0.00000000
C	14.70330436	-0.72720743	0.00000000
C	14.70330209	0.72713296	0.00000000
C	13.47800545	-1.40194004	0.00000000
C	13.47800151	1.40186196	0.00000000
C	12.25274790	-0.72720966	0.00000000
C	12.25274602	0.72712839	0.00000000
C	11.02746396	-1.40194053	0.00000000
C	11.02746076	1.40185625	0.00000000
C	9.80219336	-0.72721031	0.00000000
C	9.80219190	0.72712351	0.00000000
C	8.57691928	-1.40194164	0.00000000
C	8.57691685	1.40185250	0.00000000
C	7.35164223	-0.72721079	0.00000000
C	7.35164118	0.72711979	0.00000000
C	6.12637209	-1.40194315	0.00000000
C	6.12637044	1.40185052	0.00000000
C	4.90109376	-0.72721140	0.00000000
C	4.90109314	0.72711754	0.00000000
C	3.67582362	-1.40194446	0.00000000
C	3.67582278	1.40184976	0.00000000
C	2.45054680	-0.72721185	0.00000000
C	2.45054659	0.72711655	0.00000000
C	1.22527479	-1.40194510	0.00000000
C	1.22527476	1.40184969	0.00000000
C	0.00000048	-0.72721184	0.00000000
C	0.00000067	0.72711648	0.00000000
C	-1.22527401	-1.40194481	0.00000000
C	-1.22527326	1.40185004	0.00000000
C	-2.45054574	-0.72721123	0.00000000
C	-2.45054517	0.72711722	0.00000000
C	-3.67582263	-1.40194361	0.00000000
C	-3.67582111	1.40185081	0.00000000
C	-4.90109245	-0.72721018	0.00000000
C	-4.90109150	0.72711884	0.00000000
C	-6.12637079	-1.40194174	0.00000000
C	-6.12636852	1.40185222	0.00000000
C	-7.35164065	-0.72720902	0.00000000
C	-7.35163931	0.72712168	0.00000000
C	-8.57691773	-1.40193973	0.00000000
C	-8.57691473	1.40185476	0.00000000

C	-9.80219165	-0.72720806	0.00000000
C	-9.80218992	0.72712591	0.00000000
C	-11.02746234	-1.40193813	0.00000000
C	-11.02745866	1.40185895	0.00000000
C	-12.25274627	-0.72720697	0.00000000
C	-12.25274418	0.72713124	0.00000000
C	-13.47800402	-1.40193721	0.00000000
C	-13.47799971	1.40186503	0.00000000
C	-14.70330307	-0.72720438	0.00000000
C	-14.70330064	0.72713614	0.00000000
C	-15.92854445	-1.40193617	0.00000000
C	-15.92853957	1.40187204	0.00000000
C	-17.15385593	-0.72719737	0.00000000
C	-17.15385319	0.72713764	0.00000000
C	-18.37908993	-1.40193216	0.00000000
C	-18.37908447	1.40187711	0.00000000
C	-19.60439311	-0.72718230	0.00000000
C	-19.60439008	0.72713210	0.00000000
C	-20.82965242	-1.40192020	0.00000000
C	-20.82964636	1.40187523	0.00000000
C	-22.05490017	-0.72715765	0.00000000
C	-22.05489686	0.72711809	0.00000000
C	-23.28024614	-1.40189492	0.00000000
C	-23.28023940	1.40186117	0.00000000
C	-24.50537153	-0.72712928	0.00000000
C	-24.50536786	0.72710159	0.00000000
C	-25.73087575	-1.40185575	0.00000000
C	-25.73086824	1.40183444	0.00000000
C	-26.95583137	-0.72711659	0.00000000
C	-26.95582726	0.72710208	0.00000000
C	-28.18151503	-1.40181472	0.00000000
C	-28.18150665	1.40180725	0.00000000
C	-29.40635777	-0.72715368	0.00000000
C	-29.40635319	0.72715379	0.00000000
C	-30.63208339	-1.40180367	0.00000000
C	-30.63207414	1.40181154	0.00000000
C	-31.85708902	-0.72727714	0.00000000
C	-31.85708403	0.72729332	0.00000000
C	-33.08244284	-1.40187334	0.00000000
C	-33.08243284	1.40189802	0.00000000
C	-34.30817686	-0.72749158	0.00000000
C	-34.30817152	0.72752517	0.00000000
C	-35.53245327	-1.40207435	0.00000000
C	-35.53244274	1.40211695	0.00000000
C	-36.75965228	-0.72771210	0.00000000
C	-36.75964667	0.72776402	0.00000000
C	-37.98212200	-1.40240126	0.00000000
C	-37.98211103	1.40246259	0.00000000
C	-39.21120802	-0.72769795	0.00000000
C	-39.21120219	0.72776896	0.00000000
C	-40.43182921	-1.40269425	0.00000000
C	-40.43181778	1.40277505	0.00000000
C	-41.66195894	-0.72703568	0.00000000
C	-41.66195290	0.72712666	0.00000000
C	-42.88255075	-1.40255852	0.00000000
C	-42.88253887	1.40265963	0.00000000
C	-44.11024039	-0.72516311	0.00000000
C	-44.11023411	0.72527480	0.00000000
C	-45.33627203	-1.40107917	0.00000000
C	-45.33625975	1.40120142	0.00000000
C	-46.55385469	-0.72163979	0.00000000
C	-46.55384827	0.72177287	0.00000000
C	-47.79770285	-1.40195964	0.00000000
C	-47.79769037	1.40210372	0.00000000
C	-48.98082207	-0.70802516	0.00000000
C	-48.98081575	0.70817978	0.00000000
H	49.93509761	-1.24950551	0.00000000
H	49.93508559	1.24967781	0.00000000
H	47.78989265	-2.50077144	0.00000000
H	47.78986876	2.50092304	0.00000000
H	45.33736064	-2.50127288	0.00000000
H	45.33733713	2.50140103	0.00000000
H	42.88305886	-2.50263950	0.00000000
H	42.88303588	2.50274475	0.00000000
H	40.43174184	-2.50279115	0.00000000
H	40.43171980	2.50287437	0.00000000
H	37.98181111	-2.50252390	0.00000000
H	37.98179000	2.50258600	0.00000000
H	35.53218861	-2.50221731	0.00000000
H	35.53216831	2.50225914	0.00000000
H	33.08232409	-2.50202821	0.00000000
H	33.08230480	2.50205063	0.00000000
H	30.63208324	-2.50196316	0.00000000

H	30.63206539	2.50196736	0.00000000
H	28.18156687	-2.50197445	0.00000000
H	28.18155075	2.50196203	0.00000000
H	25.73092803	-2.50201390	0.00000000
H	25.73091369	2.50198665	0.00000000
H	23.28027720	-2.50205137	0.00000000
H	23.28026457	2.50201097	0.00000000
H	20.82966263	-2.50207546	0.00000000
H	20.82965164	2.50202349	0.00000000
H	18.37908845	-2.50208679	0.00000000
H	18.37907903	2.50202476	0.00000000
H	15.92854001	-2.50209052	0.00000000
H	15.92853190	2.50201973	0.00000000
H	13.47800137	-2.50209135	0.00000000
H	13.47799445	2.50201308	0.00000000
H	11.02746255	-2.50209199	0.00000000
H	11.02745684	2.50200750	0.00000000
H	8.57691985	-2.50209319	0.00000000
H	8.57691545	2.50200384	0.00000000
H	6.12637341	-2.50209471	0.00000000
H	6.12637036	2.50200189	0.00000000
H	3.67582466	-2.50209601	0.00000000
H	3.67582308	2.50200113	0.00000000
H	1.22527503	-2.50209664	0.00000000
H	1.22527493	2.50200107	0.00000000
H	-1.22527472	-2.50209637	0.00000000
H	-1.22527334	2.50200144	0.00000000
H	-3.67582407	-2.50209522	0.00000000
H	-3.67582125	2.50200224	0.00000000
H	-6.12637236	-2.50209340	0.00000000
H	-6.12636817	2.50200369	0.00000000
H	-8.57691838	-2.50209138	0.00000000
H	-8.57691298	2.50200621	0.00000000
H	-11.02746092	-2.50208971	0.00000000
H	-11.02745435	2.50201033	0.00000000
H	-13.47799989	-2.50208861	0.00000000
H	-13.47799229	2.50201624	0.00000000
H	-15.92853898	-2.50208738	0.00000000
H	-15.92853039	2.50202309	0.00000000
H	-18.37908797	-2.50208337	0.00000000
H	-18.37907835	2.50202816	0.00000000
H	-20.82966254	-2.50207191	0.00000000
H	-20.82965177	2.50202677	0.00000000
H	-23.28027724	-2.50204791	0.00000000
H	-23.28026517	2.50201396	0.00000000
H	-25.73092782	-2.50201079	0.00000000
H	-25.73091437	2.50198923	0.00000000
H	-28.18156613	-2.50197188	0.00000000
H	-28.18155116	2.50196414	0.00000000
H	-30.63208188	-2.50196133	0.00000000
H	-30.63206539	2.50196894	0.00000000
H	-33.08232234	-2.50202721	0.00000000
H	-33.08230449	2.50205167	0.00000000
H	-35.53218689	-2.50221721	0.00000000
H	-35.53216812	2.50225962	0.00000000
H	-37.98180995	-2.50252470	0.00000000
H	-37.98179045	2.50258584	0.00000000
H	-40.43174170	-2.50279283	0.00000000
H	-40.43172132	2.50287346	0.00000000
H	-42.88305981	-2.50264204	0.00000000
H	-42.88303863	2.50274299	0.00000000
H	-45.33736249	-2.50127622	0.00000000
H	-45.33734066	2.50139836	0.00000000
H	-47.78989510	-2.50077556	0.00000000
H	-47.78987292	2.50091950	0.00000000
H	-49.93510075	-1.24951017	0.00000000
H	-49.93508958	1.24967334	0.00000000

40-acene (triplet), E = -6167.4915735975

C	48.98155164	-0.70808647	0.00000000
C	48.98155573	0.70803100	0.00000000
C	47.79834629	-1.40202016	0.00000000
C	47.79835430	1.40197175	0.00000000
C	46.55458471	-0.72169164	0.00000000
C	46.55458885	0.72165061	0.00000000
C	45.33687682	-1.40112648	0.00000000
C	45.33688421	1.40109282	0.00000000
C	44.11092213	-0.72521628	0.00000000
C	44.11092593	0.72518929	0.00000000
C	42.88314252	-1.40259320	0.00000000
C	42.88314894	1.40257322	0.00000000
C	41.66254368	-0.72708017	0.00000000
C	41.66254696	0.72706603	0.00000000
C	40.43242143	-1.40271842	0.00000000

C	40.43242704	1.40271027	0.00000000
C	39.21168611	-0.72771941	0.00000000
C	39.21168894	0.72771599	0.00000000
C	37.98269980	-1.40241805	0.00000000
C	37.98270462	1.40241937	0.00000000
C	36.76005632	-0.72770462	0.00000000
C	36.76005854	0.72770911	0.00000000
C	35.53298548	-1.40208681	0.00000000
C	35.53298922	1.40209474	0.00000000
C	34.30855470	-0.72746229	0.00000000
C	34.30855616	0.72747182	0.00000000
C	33.08290795	-1.40188335	0.00000000
C	33.08291049	1.40189491	0.00000000
C	31.85747076	-0.72723891	0.00000000
C	31.85747155	0.72725095	0.00000000
C	30.63248136	-1.40181108	0.00000000
C	30.63248295	1.40182389	0.00000000
C	29.40674475	-0.72711561	0.00000000
C	29.40674514	0.72712820	0.00000000
C	28.18186046	-1.40181737	0.00000000
C	28.18186138	1.40182994	0.00000000
C	26.95620714	-0.72708063	0.00000000
C	26.95620726	0.72709251	0.00000000
C	25.73118534	-1.40185105	0.00000000
C	25.73118569	1.40186246	0.00000000
C	24.50571760	-0.72709267	0.00000000
C	24.50571745	0.72710319	0.00000000
C	23.28053052	-1.40188155	0.00000000
C	23.28053042	1.40189130	0.00000000
C	22.05520522	-0.72711672	0.00000000
C	22.05520495	0.72712564	0.00000000
C	20.82991437	-1.40189856	0.00000000
C	20.82991423	1.40190662	0.00000000
C	19.60465436	-0.72713467	0.00000000
C	19.60465430	0.72714247	0.00000000
C	18.37932679	-1.40190351	0.00000000
C	18.37932719	1.40191074	0.00000000
C	17.15407614	-0.72714231	0.00000000
C	17.15407657	0.72715016	0.00000000
C	15.92875187	-1.40190164	0.00000000
C	15.92875316	1.40190968	0.00000000
C	14.70348680	-0.72714232	0.00000000
C	14.70348775	0.72715167	0.00000000
C	13.47817883	-1.40189764	0.00000000
C	13.47818076	1.40190794	0.00000000
C	12.25289746	-0.72713911	0.00000000
C	12.25289860	0.72715075	0.00000000
C	11.02760356	-1.40189432	0.00000000
C	11.02760542	1.40190724	0.00000000
C	9.80231264	-0.72713600	0.00000000
C	9.80231348	0.72714952	0.00000000
C	8.57702605	-1.40189284	0.00000000
C	8.57702709	1.40190729	0.00000000
C	7.35173224	-0.72713467	0.00000000
C	7.35173237	0.72714843	0.00000000
C	6.12644752	-1.40189345	0.00000000
C	6.12644722	1.40190702	0.00000000
C	4.90115435	-0.72713547	0.00000000
C	4.90115364	0.72714700	0.00000000
C	3.67586879	-1.40189575	0.00000000
C	3.67586716	1.40190568	0.00000000
C	2.45057726	-0.72713791	0.00000000
C	2.45057587	0.72714477	0.00000000
C	1.22529004	-1.40189904	0.00000000
C	1.22528758	1.40190305	0.00000000
C	0.00000016	-0.72714111	0.00000000
C	-0.00000150	0.72714170	0.00000000
C	-1.22528887	-1.40190241	0.00000000
C	-1.22529137	1.40189956	0.00000000
C	-2.45057703	-0.72714415	0.00000000
C	-2.45057848	0.72713839	0.00000000
C	-3.67586807	-1.40190506	0.00000000
C	-3.67586984	1.40189608	0.00000000
C	-4.90115431	-0.72714648	0.00000000
C	-4.90115514	0.72713576	0.00000000
C	-6.12644751	-1.40190652	0.00000000
C	-6.12644804	1.40189353	0.00000000
C	-7.35173236	-0.72714810	0.00000000
C	-7.35173237	0.72713471	0.00000000
C	-8.57702663	-1.40190702	0.00000000
C	-8.57702591	1.40189266	0.00000000
C	-9.80231271	-0.72714950	0.00000000
C	-9.80231206	0.72713574	0.00000000

C	-11.02760422	-1.40190733	0.00000000
C	-11.02760272	1.40189385	0.00000000
C	-12.25289716	-0.72715109	0.00000000
C	-12.25289624	0.72713855	0.00000000
C	-13.47817895	-1.40190847	0.00000000
C	-13.47817748	1.40189688	0.00000000
C	-14.70348584	-0.72715247	0.00000000
C	-14.70348516	0.72714143	0.00000000
C	-15.92875100	-1.40191075	0.00000000
C	-15.92875026	1.40190054	0.00000000
C	-17.15407451	-0.72715150	0.00000000
C	-17.15407438	0.72714099	0.00000000
C	-18.37932501	-1.40191243	0.00000000
C	-18.37932524	1.40190197	0.00000000
C	-19.60465239	-0.72714441	0.00000000
C	-19.60465282	0.72713288	0.00000000
C	-20.82991234	-1.40190896	0.00000000
C	-20.82991322	1.40189654	0.00000000
C	-22.05520351	-0.72712827	0.00000000
C	-22.05520418	0.72711433	0.00000000
C	-23.28052905	-1.40189441	0.00000000
C	-23.28053003	1.40187885	0.00000000
C	-24.50571664	-0.72710661	0.00000000
C	-24.50571726	0.72708951	0.00000000
C	-25.73118502	-1.40186636	0.00000000
C	-25.73118561	1.40184752	0.00000000
C	-26.95620718	-0.72709677	0.00000000
C	-26.95620756	0.72707661	0.00000000
C	-28.18186140	-1.40183468	0.00000000
C	-28.18186147	1.40181294	0.00000000
C	-29.40674569	-0.72713332	0.00000000
C	-29.40674584	0.72711067	0.00000000
C	-30.63248351	-1.40182948	0.00000000
C	-30.63248295	1.40180569	0.00000000
C	-31.85747251	-0.72725693	0.00000000
C	-31.85747228	0.72723301	0.00000000
C	-33.08291127	-1.40190137	0.00000000
C	-33.08290985	1.40187693	0.00000000
C	-34.30855720	-0.72747875	0.00000000
C	-34.30855635	0.72745533	0.00000000
C	-35.53298992	-1.40210214	0.00000000
C	-35.53298736	1.40207928	0.00000000
C	-36.76005937	-0.72771702	0.00000000
C	-36.76005777	0.72769658	0.00000000
C	-37.98270496	-1.40242773	0.00000000
C	-37.98270132	1.40240944	0.00000000
C	-39.21168931	-0.72772487	0.00000000
C	-39.21168710	0.72771034	0.00000000
C	-40.43242680	-1.40271965	0.00000000
C	-40.43242240	1.40270878	0.00000000
C	-41.66254672	-0.72707597	0.00000000
C	-41.66254406	0.72707004	0.00000000
C	-42.88314814	-1.40258361	0.00000000
C	-42.88314288	1.40258253	0.00000000
C	-44.11092516	-0.72520026	0.00000000
C	-44.11092195	0.72520515	0.00000000
C	-45.33688294	-1.40110424	0.00000000
C	-45.33687669	1.40111480	0.00000000
C	-46.55458768	-0.72166259	0.00000000
C	-46.55458412	0.72167951	0.00000000
C	-47.79835266	-1.40198424	0.00000000
C	-47.79834581	1.40200749	0.00000000
C	-48.98155428	-0.70804402	0.00000000
C	-48.98155077	0.70807335	0.00000000
H	49.93580481	-1.24961561	0.00000000
H	49.93581210	1.24955458	0.00000000
H	47.79053390	-2.50083615	0.00000000
H	47.79054818	2.50078791	0.00000000
H	45.33796615	-2.50132384	0.00000000
H	45.33797930	2.50129048	0.00000000
H	42.88364279	-2.50267694	0.00000000
H	42.88365446	2.50265733	0.00000000
H	40.43232325	-2.50281682	0.00000000
H	40.43233337	2.50280902	0.00000000
H	37.98238527	-2.50254071	0.00000000
H	37.98239369	2.50254243	0.00000000
H	35.53272613	-2.50222815	0.00000000
H	35.53273257	2.50223656	0.00000000
H	33.08279658	-2.50203500	0.00000000
H	33.08280100	2.50204701	0.00000000
H	30.63248327	-2.50196601	0.00000000
H	30.63248598	2.50197916	0.00000000
H	28.18190707	-2.50197155	0.00000000

H	28.18190851	2.50198438	0.00000000
H	25.73122793	-2.50200312	0.00000000
H	25.73122844	2.50201474	0.00000000
H	23.28055162	-2.50203178	0.00000000
H	23.28055148	2.50204159	0.00000000
H	20.82991702	-2.50204778	0.00000000
H	20.82991691	2.50205570	0.00000000
H	18.37932066	-2.50205246	0.00000000
H	18.37932142	2.50205936	0.00000000
H	15.92874467	-2.50205064	0.00000000
H	15.92874680	2.50205834	0.00000000
H	13.47817413	-2.50204667	0.00000000
H	13.47817716	2.50205682	0.00000000
H	11.02760174	-2.50204325	0.00000000
H	11.02760453	2.50205634	0.00000000
H	8.57702612	-2.50204159	0.00000000
H	8.57702761	2.50205648	0.00000000
H	6.12644846	-2.50204208	0.00000000
H	6.12644777	2.50205619	0.00000000
H	3.67586999	-2.50204436	0.00000000
H	3.67586715	2.50205473	0.00000000
H	1.22529120	-2.50204773	0.00000000
H	1.22528689	2.50205191	0.00000000
H	-1.22528806	-2.50205123	0.00000000
H	-1.22529244	2.50204821	0.00000000
H	-3.67586789	-2.50205399	0.00000000
H	-3.67587103	2.50204457	0.00000000
H	-6.12644795	-2.50205551	0.00000000
H	-6.12644905	2.50204199	0.00000000
H	-8.57702704	-2.50205603	0.00000000
H	-8.57702615	2.50204123	0.00000000
H	-11.02760329	-2.50205626	0.00000000
H	-11.02760113	2.50204262	0.00000000
H	-13.47817527	-2.50205725	0.00000000
H	-13.47817305	2.50204581	0.00000000
H	-15.92874451	-2.50205937	0.00000000
H	-15.92874337	2.50204952	0.00000000
H	-18.37931906	-2.50206111	0.00000000
H	-18.37931940	2.50205099	0.00000000
H	-20.82991474	-2.50205817	0.00000000
H	-20.82991617	2.50204589	0.00000000
H	-23.28054974	-2.50204488	0.00000000
H	-23.28055146	2.50202925	0.00000000
H	-25.73122734	-2.50201882	0.00000000
H	-25.73122852	2.50199977	0.00000000
H	-28.18190807	-2.50198927	0.00000000
H	-28.18190842	2.50196727	0.00000000
H	-30.63248608	-2.50198484	0.00000000
H	-30.63248523	2.50196071	0.00000000
H	-33.08280130	-2.50205349	0.00000000
H	-33.08279891	2.50202859	0.00000000
H	-35.53273280	-2.50224392	0.00000000
H	-35.53272847	2.50222058	0.00000000
H	-37.98239358	-2.50255070	0.00000000
H	-37.98238725	2.50253200	0.00000000
H	-40.43233268	-2.50281827	0.00000000
H	-40.43232471	2.50280705	0.00000000
H	-42.88365322	-2.50266760	0.00000000
H	-42.88364363	2.50266615	0.00000000
H	-45.33797762	-2.50130181	0.00000000
H	-45.33796650	2.50131207	0.00000000
H	-47.79054607	-2.50080032	0.00000000
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42-acene (singlet), E = -6471.9766375938

C	51.43129676	-0.70806728	0.00000000
C	51.43129382	0.70814287	0.00000000
C	50.24817553	-1.40198947	0.00000000
C	50.24816972	1.40206020	0.00000000
C	49.00432687	-0.72167659	0.00000000
C	49.00432389	0.72174218	0.00000000
C	47.78674525	-1.40111064	0.00000000
C	47.78673949	1.40117131	0.00000000
C	46.56070183	-0.72518099	0.00000000
C	46.56069884	0.72523661	0.00000000
C	45.33301945	-1.40259330	0.00000000
C	45.33301376	1.40264404	0.00000000
C	44.11243475	-0.72705380	0.00000000
C	44.11243182	0.72709957	0.00000000
C	42.88231405	-1.40271112	0.00000000
C	42.88230855	1.40275213	0.00000000
C	41.66168403	-0.72771159	0.00000000

C	41.66168123	0.72774783	0.00000000
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C	-41.66218157	-0.72772253	0.00000000
C	-41.66217965	0.72770591	0.00000000
C	-42.88291386	-1.40271824	0.00000000
C	-42.88291035	1.40270464	0.00000000
C	-44.11302224	-0.72707302	0.00000000
C	-44.11301998	0.72706354	0.00000000
C	-45.33361381	-1.40259662	0.00000000
C	-45.33360991	1.40259116	0.00000000
C	-46.56137158	-0.72519310	0.00000000
C	-46.56136914	0.72519224	0.00000000
C	-47.78734755	-1.40111046	0.00000000
C	-47.78734323	1.40111406	0.00000000
C	-49.00503636	-0.72167307	0.00000000
C	-49.00503388	0.72168120	0.00000000
C	-50.24880982	-1.40198493	0.00000000
C	-50.24880521	1.40199759	0.00000000
C	-51.43200358	-0.70805650	0.00000000
C	-51.43200120	0.70807334	0.00000000
H	52.38625520	-1.24962221	0.00000000
H	52.38626086	1.24956513	0.00000000
H	50.24097385	-2.50083091	0.00000000

H	50.24098499	2.50078376	0.00000000
H	47.78837474	-2.50132527	0.00000000
H	47.78838543	2.50128995	0.00000000
H	45.33411015	-2.50268536	0.00000000
H	45.33412008	2.50266191	0.00000000
H	42.88282892	-2.50281374	0.00000000
H	42.88283790	2.50280111	0.00000000
H	40.43288941	-2.50253897	0.00000000
H	40.43289714	2.50253531	0.00000000
H	37.98323324	-2.50222800	0.00000000
H	37.98323928	2.50223059	0.00000000
H	35.53331125	-2.50203551	0.00000000
H	35.53331558	2.50204126	0.00000000
H	33.08300999	-2.50196651	0.00000000
H	33.08301297	2.50197305	0.00000000
H	30.63244496	-2.50197247	0.00000000
H	30.63244714	2.50197855	0.00000000
H	28.18177452	-2.50200441	0.00000000
H	28.18177626	2.50200980	0.00000000
H	25.73110424	-2.50203342	0.00000000
H	25.73110565	2.50203816	0.00000000
H	23.28047380	-2.50204970	0.00000000
H	23.28047509	2.50205397	0.00000000
H	20.82988050	-2.50205472	0.00000000
H	20.82988196	2.50205902	0.00000000
H	18.37930684	-2.50205350	0.00000000
H	18.37930875	2.50205870	0.00000000
H	15.92873776	-2.50205024	0.00000000
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H	13.47816608	-2.50204720	0.00000000
H	13.47816857	2.50205678	0.00000000
H	11.02759104	-2.50204531	0.00000000
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H	8.57701437	-2.50204482	0.00000000
H	8.57701523	2.50205722	0.00000000
H	6.12643789	-2.50204564	0.00000000
H	6.12643741	2.50205675	0.00000000
H	3.67586238	-2.50204757	0.00000000
H	3.67586064	2.50205531	0.00000000
H	1.22528761	-2.50205015	0.00000000
H	1.22528510	2.50205296	0.00000000
H	-1.22528709	-2.50205288	0.00000000
H	-1.22528967	2.50205010	0.00000000
H	-3.67586237	-2.50205519	0.00000000
H	-3.67586436	2.50204732	0.00000000
H	-6.12643867	-2.50205670	0.00000000
H	-6.12643960	2.50204513	0.00000000
H	-8.57701594	-2.50205733	0.00000000
H	-8.57701563	2.50204398	0.00000000
H	-11.02759291	-2.50205738	0.00000000
H	-11.02759175	2.50204412	0.00000000
H	-13.47816770	-2.50205764	0.00000000
H	-13.47816628	2.50204559	0.00000000
H	-15.92873857	-2.50205886	0.00000000
H	-15.92873743	2.50204814	0.00000000
H	-18.37930670	-2.50206104	0.00000000
H	-18.37930616	2.50205089	0.00000000
H	-20.82987966	-2.50206226	0.00000000
H	-20.82987974	2.50205158	0.00000000
H	-23.28047283	-2.50205822	0.00000000
H	-23.28047331	2.50204593	0.00000000
H	-25.73110376	-2.50204347	0.00000000
H	-25.73110429	2.50202888	0.00000000
H	-28.18177492	-2.50201617	0.00000000
H	-28.18177531	2.50199894	0.00000000
H	-30.63244640	-2.50198598	0.00000000
H	-30.63244655	2.50196585	0.00000000
H	-33.08301276	-2.50198149	0.00000000
H	-33.08301217	2.50195859	0.00000000
H	-35.53331555	-2.50205071	0.00000000
H	-35.53331370	2.50202615	0.00000000
H	-37.98323900	-2.50224101	0.00000000
H	-37.98323557	2.50221717	0.00000000
H	-40.43289625	-2.50254682	0.00000000
H	-40.43289119	2.50252663	0.00000000
H	-42.88283617	-2.50281382	0.00000000
H	-42.88282988	2.50280000	0.00000000
H	-45.33411747	-2.50267596	0.00000000
H	-45.33411026	2.50267032	0.00000000
H	-47.78838199	-2.50130545	0.00000000
H	-47.78837412	2.50130893	0.00000000
H	-50.24098093	-2.50080072	0.00000000
H	-50.24097260	2.50081330	0.00000000

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H	-52.38625304	1.24960360	0.00000000
44-acene (singlet), E = -6776.4596960782			
C	53.88178871	-0.70827197	0.00000000
C	53.88180003	0.70793847	0.00000000
C	52.69865699	-1.40218244	0.00000000
C	52.69867937	1.40186779	0.00000000
C	51.45481288	-0.72186324	0.00000000
C	51.45482442	0.72156839	0.00000000
C	50.23723112	-1.40127674	0.00000000
C	50.23725340	1.40100125	0.00000000
C	49.01118457	-0.72534352	0.00000000
C	49.01119607	0.72508742	0.00000000
C	47.78351022	-1.40273774	0.00000000
C	47.78353232	1.40250106	0.00000000
C	46.56290944	-0.72718396	0.00000000
C	46.56292081	0.72696639	0.00000000
C	45.33279753	-1.40283660	0.00000000
C	45.33281928	1.40263816	0.00000000
C	44.11216797	-0.72781591	0.00000000
C	44.11217914	0.72763628	0.00000000
C	42.88309210	-1.40251241	0.00000000
C	42.88311337	1.40235151	0.00000000
C	41.66062172	-0.72780229	0.00000000
C	41.66063262	0.72765974	0.00000000
C	40.43342327	-1.40215768	0.00000000
C	40.43344391	1.40203335	0.00000000
C	39.20915488	-0.72755632	0.00000000
C	39.20916543	0.72744983	0.00000000
C	37.98341455	-1.40193041	0.00000000
C	37.98343450	1.40184149	0.00000000
C	36.75807381	-0.72731685	0.00000000
C	36.75808397	0.72724521	0.00000000
C	35.53305947	-1.40183526	0.00000000
C	35.53307868	1.40178052	0.00000000
C	34.30734773	-0.72716904	0.00000000
C	34.30735752	0.72713094	0.00000000
C	33.08249763	-1.40182257	0.00000000
C	33.08251604	1.40180071	0.00000000
C	31.85682652	-0.72710861	0.00000000
C	31.85683584	0.72710259	0.00000000
C	30.63186707	-1.40184046	0.00000000
C	30.63188443	1.40184988	0.00000000
C	29.40637345	-0.72710031	0.00000000
C	29.40638214	0.72712448	0.00000000
C	28.18124431	-1.40185962	0.00000000
C	28.18126026	1.40189814	0.00000000
C	26.95590811	-0.72710810	0.00000000
C	26.95591597	0.72716001	0.00000000
C	25.73065907	-1.40186678	0.00000000
C	25.73067333	1.40193167	0.00000000
C	24.50540896	-0.72711485	0.00000000
C	24.50541589	0.72719163	0.00000000
C	23.28010507	-1.40186124	0.00000000
C	23.28011755	1.40194945	0.00000000
C	22.05487966	-0.72711431	0.00000000
C	22.05488569	0.72721295	0.00000000
C	20.82956799	-1.40185119	0.00000000
C	20.82957883	1.40195971	0.00000000
C	19.60433536	-0.72710785	0.00000000
C	19.60434060	0.72722550	0.00000000
C	18.37903558	-1.40183917	0.00000000
C	18.37904502	1.40196533	0.00000000
C	17.15378603	-0.72709777	0.00000000
C	17.15379061	0.72723201	0.00000000
C	15.92850174	-1.40182742	0.00000000
C	15.92851005	1.40196903	0.00000000
C	14.70324077	-0.72708767	0.00000000
C	14.70324484	0.72723646	0.00000000
C	13.47796846	-1.40182006	0.00000000
C	13.47797583	1.40197531	0.00000000
C	12.25269940	-0.72708127	0.00000000
C	12.25270299	0.72724294	0.00000000
C	11.02742978	-1.40181553	0.00000000
C	11.02743624	1.40198284	0.00000000
C	9.80215736	-0.72707480	0.00000000
C	9.80216046	0.72724773	0.00000000
C	8.57688956	-1.40181081	0.00000000
C	8.57689500	1.40198850	0.00000000
C	7.35161766	-0.72706968	0.00000000
C	7.35162018	0.72725201	0.00000000
C	6.12634941	-1.40180762	0.00000000
C	6.12635360	1.40199370	0.00000000

C	4.90107879	-0.72706617	0.00000000
C	4.90108059	0.72725571	0.00000000
C	3.67580947	-1.40180489	0.00000000
C	3.67581215	1.40199697	0.00000000
C	2.45053952	-0.72706411	0.00000000
C	2.45054047	0.72725825	0.00000000
C	1.22526982	-1.40180355	0.00000000
C	1.22527075	1.40199877	0.00000000
C	0.00000009	-0.72706346	0.00000000
C	0.00000010	0.72725922	0.00000000
C	-1.22526963	-1.40180351	0.00000000
C	-1.22527054	1.40199878	0.00000000
C	-2.45053928	-0.72706406	0.00000000
C	-2.45054022	0.72725825	0.00000000
C	-3.67580917	-1.40180482	0.00000000
C	-3.67581183	1.40199696	0.00000000
C	-4.90107841	-0.72706610	0.00000000
C	-4.90108020	0.72725573	0.00000000
C	-6.12634893	-1.40180754	0.00000000
C	-6.12635313	1.40199371	0.00000000
C	-7.35161711	-0.72706963	0.00000000
C	-7.35161962	0.72725202	0.00000000
C	-8.57688895	-1.40181078	0.00000000
C	-8.57689439	1.40198850	0.00000000
C	-9.80215672	-0.72707479	0.00000000
C	-9.80215982	0.72724774	0.00000000
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C	-11.02743561	1.40198288	0.00000000
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C	-13.47796796	-1.40182012	0.00000000
C	-13.47797535	1.40197538	0.00000000
C	-14.70324042	-0.72708773	0.00000000
C	-14.70324450	0.72723651	0.00000000
C	-15.92850157	-1.40182754	0.00000000
C	-15.92850991	1.40196911	0.00000000
C	-17.15378610	-0.72709788	0.00000000
C	-17.15379068	0.72723204	0.00000000
C	-18.37903584	-1.40183934	0.00000000
C	-18.37904530	1.40196536	0.00000000
C	-19.60433583	-0.72710799	0.00000000
C	-19.60434107	0.72722549	0.00000000
C	-20.82956864	-1.40185135	0.00000000
C	-20.82957949	1.40195970	0.00000000
C	-22.05488046	-0.72711444	0.00000000
C	-22.05488649	0.72721289	0.00000000
C	-23.28010597	-1.40186137	0.00000000
C	-23.28011846	1.40194938	0.00000000
C	-24.50540990	-0.72711496	0.00000000
C	-24.50541684	0.72719153	0.00000000
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C	-25.73067426	1.40193154	0.00000000
C	-26.95590895	-0.72710815	0.00000000
C	-26.95591681	0.72715987	0.00000000
C	-28.18124501	-1.40185961	0.00000000
C	-28.18126096	1.40189796	0.00000000
C	-29.40637395	-0.72710032	0.00000000
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C	-30.63186733	-1.40184042	0.00000000
C	-30.63188468	1.40184966	0.00000000
C	-31.85682650	-0.72710859	0.00000000
C	-31.85683583	0.72710242	0.00000000
C	-33.08249735	-1.40182250	0.00000000
C	-33.08251576	1.40180051	0.00000000
C	-34.30734719	-0.72716901	0.00000000
C	-34.30735697	0.72713080	0.00000000
C	-35.53305869	-1.40183523	0.00000000
C	-35.53307790	1.40178036	0.00000000
C	-36.75807285	-0.72731687	0.00000000
C	-36.75808302	0.72724509	0.00000000
C	-37.98341349	-1.40193043	0.00000000
C	-37.98343341	1.40184142	0.00000000
C	-39.20915378	-0.72755638	0.00000000
C	-39.20916431	0.72744979	0.00000000
C	-40.43342221	-1.40215777	0.00000000
C	-40.43344282	1.40203337	0.00000000
C	-41.66062079	-0.72780237	0.00000000
C	-41.66063166	0.72765979	0.00000000
C	-42.88309137	-1.40251255	0.00000000
C	-42.88311261	1.40235162	0.00000000
C	-44.11216747	-0.72781599	0.00000000
C	-44.11217864	0.72763640	0.00000000
C	-45.33279733	-1.40283673	0.00000000

C	-45.33281906	1.40263835	0.00000000
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C	-49.01119673	0.72508761	0.00000000
C	-50.23723204	-1.40127680	0.00000000
C	-50.23725427	1.40100151	0.00000000
C	-51.45481398	-0.72186322	0.00000000
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C	-52.69865827	-1.40218242	0.00000000
C	-52.69868059	1.40186803	0.00000000
C	-53.88179009	-0.70827187	0.00000000
C	-53.88180138	0.70793868	0.00000000
H	54.83606325	-1.24980175	0.00000000
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H	52.69087017	2.50068373	0.00000000
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H	50.23827807	2.50119836	0.00000000
H	47.78396341	-2.50281854	0.00000000
H	47.78400285	2.50258191	0.00000000
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H	45.33272471	2.50273401	0.00000000
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H	35.53308620	2.50193560	0.00000000
H	33.08254364	-2.50197689	0.00000000
H	33.08257641	2.50195516	0.00000000
H	30.63191474	-2.50199264	0.00000000
H	30.63194561	2.50200229	0.00000000
H	28.18126620	-2.50200982	0.00000000
H	28.18129458	2.50204868	0.00000000
H	25.73066216	-2.50201572	0.00000000
H	25.73068761	2.50208099	0.00000000
H	23.28009840	-2.50200985	0.00000000
H	23.28012073	2.50209840	0.00000000
H	20.82955814	-2.50199980	0.00000000
H	20.82957754	2.50210855	0.00000000
H	18.37902768	-2.50198828	0.00000000
H	18.37904459	2.50211454	0.00000000
H	15.92849803	-2.50197643	0.00000000
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H	13.47798309	2.50212463	0.00000000
H	11.02742948	-2.50196507	0.00000000
H	11.02744103	2.50213231	0.00000000
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H	6.12634724	-2.50195718	0.00000000
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H	3.67580832	-2.50195446	0.00000000
H	3.67581309	2.50214671	0.00000000
H	1.22526954	-2.50195312	0.00000000
H	1.22527121	2.50214858	0.00000000
H	-1.22526939	-2.50195308	0.00000000
H	-1.22527102	2.50214857	0.00000000
H	-3.67580804	-2.50195437	0.00000000
H	-3.67581278	2.50214667	0.00000000
H	-6.12634678	-2.50195709	0.00000000
H	-6.12635427	2.50214332	0.00000000
H	-8.57688661	-2.50196045	0.00000000
H	-8.57689633	2.50213816	0.00000000
H	-11.02742882	-2.50196513	0.00000000
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H	-13.47796941	-2.50196959	0.00000000
H	-13.47798260	2.50212476	0.00000000
H	-15.92849783	-2.50197664	0.00000000
H	-15.92851275	2.50211820	0.00000000
H	-18.37902789	-2.50198853	0.00000000
H	-18.37904486	2.50211466	0.00000000
H	-20.82955874	-2.50200004	0.00000000
H	-20.82957818	2.50210862	0.00000000
H	-23.28009926	-2.50201000	0.00000000
H	-23.28012162	2.50209835	0.00000000
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H	-28.18129529	2.50204841	0.00000000
H	-30.63191501	-2.50199248	0.00000000
H	-30.63194586	2.50200195	0.00000000
H	-33.08254339	-2.50197670	0.00000000
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H	-35.53305121	-2.50199014	0.00000000
H	-35.53308546	2.50193536	0.00000000
H	-37.98328863	-2.50208171	0.00000000
H	-37.98332416	2.50199277	0.00000000
H	-40.43315337	-2.50229819	0.00000000
H	-40.43319012	2.50217388	0.00000000
H	-42.88277238	-2.50263350	0.00000000
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H	-45.33268574	-2.50293266	0.00000000
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H	-47.78396383	-2.50281880	0.00000000
H	-47.78400318	2.50258229	0.00000000
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44-acene (triplet), E = -6776.4578785439

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C	49.01178780	-0.72520553	0.00000000
C	49.01178824	0.72519661	0.00000000
C	47.78405152	-1.40260121	0.00000000
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H	-8.57694825	-2.50203337	0.00000000
H	-8.57694568	2.50205892	0.00000000
H	-11.02750941	-2.50203360	0.00000000
H	-11.02750917	2.50205860	0.00000000
H	-13.47807243	-2.50203324	0.00000000
H	-13.47807386	2.50205539	0.00000000
H	-15.92862247	-2.50203484	0.00000000
H	-15.92862463	2.50205294	0.00000000
H	-18.37917838	-2.50204010	0.00000000
H	-18.37918033	2.50205418	0.00000000
H	-20.82973260	-2.50204444	0.00000000

H	-20.82973373	2.50205552	0.00000000
H	-23.28028595	-2.50204802	0.00000000
H	-23.28028606	2.50205756	0.00000000
H	-25.73084397	-2.50205100	0.00000000
H	-25.73084334	2.50206029	0.00000000
H	-28.18142438	-2.50204633	0.00000000
H	-28.18142362	2.50205597	0.00000000
H	-30.63205509	-2.50203039	0.00000000
H	-30.63205495	2.50204009	0.00000000
H	-33.08271630	-2.50200375	0.00000000
H	-33.08271737	2.50201229	0.00000000
H	-35.53337848	-2.50197433	0.00000000
H	-35.53338106	2.50197980	0.00000000
H	-37.98393726	-2.50197242	0.00000000
H	-37.98394104	2.50197283	0.00000000
H	-40.43423358	-2.50204552	0.00000000
H	-40.43423777	2.50203973	0.00000000
H	-42.88414965	-2.50224115	0.00000000
H	-42.88415342	2.50222951	0.00000000
H	-45.33379702	-2.50255413	0.00000000
H	-45.33379969	2.50253839	0.00000000
H	-47.78371571	-2.50283000	0.00000000
H	-47.78371706	2.50281262	0.00000000
H	-50.23499399	-2.50269264	0.00000000
H	-50.23499438	2.50267559	0.00000000
H	-52.68928394	-2.50132396	0.00000000
H	-52.68928400	2.50130801	0.00000000
H	-55.14189780	-2.50082427	0.00000000
H	-55.14189791	2.50080899	0.00000000
H	-57.28717033	-1.24962520	0.00000000
H	-57.28717038	1.24960991	0.00000000

TABLES

TABLE S1. Comparison of errors (in kcal/mol) of the reaction energies (in kcal/mol) of 30 chemical reactions [1], calculated by TAO-LDA (with various θ (in mHartree)). The $\theta=0$ case corresponds to KS-LDA.

Reactions	ΔE_{ref}	$\theta=0$	$\theta=1$	$\theta=3$	$\theta=5$	$\theta=7$	$\theta=10$	$\theta=15$	$\theta=20$	$\theta=30$	$\theta=40$
H + N ₂ O → OH + N ₂	-65.08	35.68	35.59	33.88	32.18	30.50	28.01	23.95	20.08	13.35	7.96
H + FCH ₃ → HF + CH ₃	-26.64	8.28	8.28	8.30	8.34	8.39	8.49	8.69	8.84	8.39	6.57
H + F ₂ → HF + F	-103.91	18.54	17.66	15.26	12.86	10.46	6.89	1.43	-2.85	-7.37	-7.75
CH ₃ + FCl → CH ₃ F + Cl	-52.74	3.57	1.52	-0.89	-3.30	-5.71	-9.25	-14.43	-18.04	-20.03	-16.64
F ⁻ + CH ₃ Cl → FCH ₃ + Cl ⁻	-32.65	-0.90	-0.89	-0.84	-0.74	-0.62	-0.40	0.03	0.36	0.50	0.84
F ⁻ ···CH ₃ Cl → FCH ₃ ···Cl ⁻	-26.73	4.05	4.05	4.07	4.11	4.18	4.37	5.13	6.33	9.32	13.16
OH ⁻ + CH ₃ F → HOCH ₃ + F ⁻	-20.11	0.05	0.05	0.01	-0.04	-0.07	0.12	1.38	3.44	8.03	11.54
OH ⁻ ···CH ₃ F → HOCH ₃ ···F ⁻	-36.24	-7.90	-7.90	-7.96	-8.03	-8.07	-7.86	-6.85	-5.56	-3.49	-2.21
H + N ₂ → HN ₂	3.97	-15.60	-15.61	-15.65	-15.73	-15.92	-16.55	-18.63	-21.78	-30.14	-39.72
H + CO → HCO	-19.51	-14.40	-14.41	-14.46	-14.56	-14.74	-15.31	-17.22	-20.13	-27.44	-35.05
H + C ₂ H ₄ → CH ₃ CH ₂	-40.03	-4.52	-4.52	-4.58	-4.67	-4.79	-5.04	-5.63	-6.44	-8.76	-11.82
CH ₃ + C ₂ H ₄ → CH ₃ CH ₂ CH ₂	-26.12	-12.64	-12.65	-12.73	-12.88	-13.09	-13.50	-14.45	-15.72	-18.75	-21.52
HCN → HNC	15.05	-0.83	-0.82	-0.81	-0.79	-0.77	-0.72	-0.62	-0.58	-0.90	-1.64
H + HCl → H ₂ + Cl	-3.0	11.13	9.08	6.70	4.35	2.01	-1.46	-7.17	-12.73	-22.94	-31.21
OH + H ₂ → H + H ₂ O	-16.1	-13.62	-13.52	-11.82	-10.12	-8.43	-5.94	-1.86	2.10	9.59	16.41
CH ₃ + H ₂ → H + CH ₄	-3.2	-7.09	-7.09	-7.12	-7.17	-7.25	-7.38	-7.67	-7.90	-7.50	-5.37
OH + CH ₄ → CH ₃ + H ₂ O	-12.9	-6.53	-6.43	-4.69	-2.94	-1.19	1.44	5.80	10.00	17.09	21.78
OH + NH ₃ → H ₂ O + NH ₂	-9.5	-3.67	-3.57	-1.84	-0.11	1.58	3.91	6.99	9.23	12.27	14.40
HCl + CH ₃ → Cl + CH ₄	-6.2	4.04	1.98	-0.42	-2.82	-5.23	-8.84	-14.83	-20.63	-30.44	-36.58
OH + C ₂ H ₆ → H ₂ O + C ₂ H ₅	-16.5	-9.27	-9.17	-7.44	-5.68	-3.93	-1.30	3.02	7.04	13.18	16.45
F + H ₂ → HF + H	-31.6	-18.31	-17.43	-15.06	-12.70	-10.36	-6.87	-1.14	4.50	15.39	25.45
O + CH ₄ → OH + CH ₃	5.6	-7.02	-7.10	-7.58	-6.91	-6.23	-5.21	-3.52	-1.98	-0.21	-1.05
H + PH ₃ → PH ₂ + H ₂	-20.1	3.51	3.51	3.54	3.58	3.63	3.64	3.25	2.18	-1.39	-5.53
H + HO → H ₂ + O	-2.4	14.11	14.20	14.70	14.08	13.48	12.59	11.19	9.88	7.71	6.42
H + H ₂ S → H ₂ + HS	-13.8	7.93	6.92	5.21	3.51	1.84	-0.64	-4.67	-8.49	-15.06	-20.09
O + HCl → OH + Cl	-0.6	-2.98	-5.12	-8.00	-9.73	-11.46	-14.05	-18.36	-22.61	-30.65	-37.63
NH ₂ + CH ₃ → CH ₄ + NH	-14.4	3.87	3.87	3.86	3.84	3.85	4.05	4.95	6.27	9.44	13.43
NH ₂ + C ₂ H ₅ → C ₂ H ₆ + NH	-10.8	6.62	6.61	6.60	6.58	6.59	6.79	7.73	9.23	13.34	18.77
C ₂ H ₆ + NH ₂ → NH ₃ + C ₂ H ₅	-7.0	-5.61	-5.60	-5.59	-5.57	-5.51	-5.20	-3.97	-2.19	0.92	2.05
NH ₂ + CH ₄ → CH ₃ + NH ₃	-3.3	-2.96	-2.96	-2.95	-2.93	-2.87	-2.56	-1.29	0.67	4.72	7.29
MSE		-0.41	-0.72	-0.94	-1.13	-1.32	-1.59	-1.96	-2.25	-2.73	-3.04
MAE		8.51	8.27	7.75	7.36	7.09	6.95	7.53	8.92	12.28	15.21
rms		11.10	10.89	10.31	9.76	9.38	9.16	9.75	11.25	15.20	19.03
Max(-)		-18.31	-17.43	-15.65	-15.73	-15.92	-16.55	-18.63	-22.61	-30.65	-39.72
Max(+)		35.68	35.59	33.88	32.18	30.50	28.01	23.95	20.08	17.09	25.45

TABLE S2. The 166 experimentally determined equilibrium bond lengths (in Å) of 136 molecules included in EXTS [2]. Optimized bond lengths are calculated by TAO-LDA (with various θ (in mHartree)). The $\theta=0$ case corresponds to KS-LDA.

Molecule	Experiment	$\theta=0$	$\theta=1$	$\theta=3$	$\theta=5$	$\theta=7$	$\theta=10$	$\theta=15$	$\theta=20$	$\theta=30$	$\theta=40$
H ₂ N ⁻	1.028	1.037	1.037	1.037	1.037	1.037	1.037	1.037	1.036	1.034	1.033
NO ⁻ (³ Σ ⁻)	1.258	1.250	1.250	1.250	1.250	1.250	1.249	1.242	1.234	1.222	1.219
PO ⁻ (³ Σ ⁻)	1.540	1.539	1.539	1.539	1.539	1.539	1.537	1.534	1.532	1.537	1.551
BeH ⁺ (¹ Σ ⁺)	1.312	1.337	1.337	1.337	1.337	1.336	1.335	1.334	1.337	1.349	1.364

CH ⁺ (¹ Σ ⁺)	1.131	1.162	1.162	1.161	1.161	1.162	1.163	1.165	1.166	1.168	1.168
CN ⁺ (¹ Σ ⁺)	1.173	1.173	1.177	1.188	1.196	1.203	1.210	1.219	1.224	1.227	1.226
H ₃ ⁺	0.877	0.906	0.906	0.906	0.906	0.906	0.905	0.904	0.903	0.899	0.895
H ₃ O ⁺	0.976	0.990	0.990	0.990	0.990	0.990	0.990	0.989	0.989	0.987	0.986
HCO ⁺	1.097 (CH)	1.111	1.111	1.111	1.111	1.111	1.110	1.110	1.109	1.106	1.103
	1.105 (CO)	1.105	1.105	1.105	1.105	1.105	1.105	1.105	1.105	1.105	1.109
MgH ⁺ (¹ Σ ⁺)	1.652	1.671	1.671	1.670	1.670	1.669	1.668	1.669	1.675	1.695	1.717
NO ⁺ (¹ Σ ⁺)	1.063	1.062	1.062	1.062	1.062	1.062	1.062	1.061	1.061	1.062	1.065
NS ⁺ (¹ Σ ⁺)	1.440	1.433	1.433	1.433	1.433	1.433	1.433	1.432	1.433	1.441	1.459
OH ⁺ (³ Σ ⁻)	1.029	1.055	1.055	1.055	1.055	1.055	1.055	1.055	1.057	1.062	1.068
SiH ⁺ (¹ Σ ⁺)	1.504	1.538	1.538	1.538	1.538	1.537	1.538	1.542	1.546	1.551	1.551
NH ₄ ⁺	1.021	1.035	1.035	1.035	1.035	1.034	1.034	1.034	1.033	1.031	1.029
AlCl (¹ Σ ⁺)	2.130	2.136	2.136	2.136	2.136	2.135	2.135	2.133	2.131	2.134	2.151
AlF (¹ Σ ⁺)	1.654	1.669	1.669	1.669	1.669	1.669	1.669	1.668	1.668	1.667	1.672
AlH (¹ Σ ⁺)	1.648	1.680	1.680	1.680	1.679	1.679	1.677	1.671	1.664	1.648	1.636
AlN (³ Π _i)	1.786	1.769	1.769	1.768	1.770	1.774	1.781	1.787	1.790	1.792	1.796
BCl (¹ Σ ⁺)	1.797	1.706	1.706	1.706	1.706	1.706	1.706	1.702	1.697	1.687	1.687
BeO (¹ Σ ⁺)	1.331	1.326	1.326	1.326	1.327	1.331	1.338	1.348	1.355	1.367	1.377
BeS (¹ Σ ⁺)	1.742	1.739	1.739	1.739	1.744	1.753	1.766	1.783	1.796	1.815	1.834
BF (¹ Σ ⁺)	1.263	1.256	1.256	1.256	1.256	1.256	1.256	1.256	1.257	1.261	1.265
BF ₃	1.307	1.307	1.307	1.307	1.307	1.307	1.306	1.306	1.305	1.304	1.304
BH (¹ Σ ⁺)	1.232	1.256	1.256	1.256	1.255	1.254	1.251	1.243	1.236	1.225	1.216
BN (³ Π)	1.281	1.323	1.323	1.322	1.322	1.322	1.321	1.317	1.315	1.316	1.324
C ₆ H ₆	1.390 (CC)	1.385	1.385	1.385	1.385	1.385	1.385	1.384	1.384	1.386	1.388
	1.086 (CH)	1.094	1.094	1.094	1.093	1.093	1.093	1.092	1.091	1.089	1.087
CCl ₂ O	1.177 (CO)	1.177	1.177	1.177	1.177	1.177	1.177	1.178	1.179	1.185	1.193
	1.737 (CCl)	1.731	1.731	1.730	1.730	1.730	1.729	1.728	1.727	1.729	1.743
CF ₄	1.315	1.318	1.318	1.317	1.317	1.317	1.317	1.317	1.316	1.314	1.314
CH ₂ Cl ₂	1.766 (CCl)	1.754	1.754	1.754	1.754	1.754	1.753	1.752	1.752	1.759	1.779
	1.080 (CH)	1.096	1.096	1.096	1.096	1.095	1.095	1.094	1.094	1.092	1.090
CH ₂ F ₂	1.351 (CF)	1.348	1.348	1.348	1.348	1.348	1.348	1.348	1.347	1.346	1.346
	1.084 (CH)	1.105	1.105	1.105	1.105	1.105	1.104	1.103	1.102	1.100	1.098
CH ₂ O ₂ (<i>trans</i>)	1.201 (C=O)	1.198	1.198	1.198	1.198	1.198	1.198	1.198	1.199	1.204	1.213
	1.091 (CH)	1.111	1.111	1.110	1.110	1.110	1.110	1.109	1.107	1.103	1.098
	1.340 (CO)	1.332	1.332	1.332	1.332	1.332	1.332	1.331	1.331	1.330	1.330
	0.969 (OH)	0.983	0.983	0.983	0.983	0.983	0.983	0.982	0.982	0.980	0.981
CH ₃ Cl	1.086 (CH)	1.096	1.096	1.096	1.096	1.096	1.096	1.095	1.094	1.092	1.090
	1.778 (CCl)	1.763	1.763	1.763	1.763	1.762	1.762	1.761	1.760	1.767	1.788
CH ₃ F	1.086 (CH)	1.102	1.102	1.102	1.102	1.102	1.101	1.100	1.099	1.097	1.095
	1.383 (CF)	1.371	1.371	1.371	1.371	1.371	1.371	1.370	1.370	1.369	1.371
CH ₄	1.087	1.097	1.097	1.097	1.097	1.097	1.096	1.095	1.094	1.092	1.089
CHF ₃	1.328 (CF)	1.330	1.330	1.330	1.330	1.330	1.330	1.329	1.329	1.327	1.327
	1.091 (CH)	1.105	1.105	1.105	1.105	1.105	1.104	1.104	1.103	1.100	1.098
Cl ₂ (¹ Σ _g ⁺)	1.988	1.980	1.980	1.980	1.980	1.979	1.982	2.000	2.041	2.210	2.569
ClCN	1.629 (CCl)	1.612	1.612	1.612	1.612	1.612	1.611	1.610	1.610	1.611	1.618
	1.160 (CN)	1.160	1.160	1.160	1.160	1.160	1.160	1.159	1.159	1.162	1.171
ClF	1.628	1.625	1.625	1.625	1.625	1.625	1.626	1.636	1.661	1.756	1.983
CO (¹ Σ ⁺)	1.128	1.127	1.127	1.127	1.127	1.127	1.127	1.127	1.127	1.128	1.133
CO ₂	1.160	1.162	1.162	1.162	1.162	1.161	1.161	1.161	1.161	1.161	1.164
CS (¹ Σ ⁺)	1.535	1.533	1.533	1.533	1.533	1.533	1.532	1.532	1.532	1.540	1.558
CS ₂	1.553	1.551	1.551	1.551	1.551	1.550	1.550	1.550	1.552	1.558	1.568
F ₂ (¹ Σ _g ⁺)	1.412	1.383	1.383	1.383	1.383	1.383	1.383	1.393	1.423	1.601	1.929

F ₂ O	1.405	1.388	1.388	1.388	1.388	1.388	1.388	1.393	1.404	1.324	1.335
F ₂ S	1.587	1.598	1.598	1.598	1.598	1.598	1.598	1.601	1.607	1.621	1.643
F ₂ Si	1.590	1.607	1.607	1.607	1.607	1.607	1.607	1.606	1.605	1.605	1.607
F ₃ HSi	1.562 (SiF)	1.575	1.575	1.575	1.575	1.575	1.574	1.574	1.573	1.571	1.572
	1.447 (SiH)	1.470	1.470	1.470	1.469	1.469	1.468	1.467	1.465	1.461	1.459
H ₂ (¹ Σ _g ⁺)	0.741	0.766	0.766	0.766	0.766	0.766	0.765	0.764	0.762	0.759	0.756
H ₂ CCCH ₂	1.076 (CH)	1.095	1.095	1.094	1.094	1.094	1.094	1.093	1.092	1.091	1.090
	1.308 (CC)	1.298	1.298	1.298	1.298	1.298	1.298	1.297	1.297	1.300	1.306
H ₂ CS	1.611 (CS)	1.601	1.601	1.601	1.601	1.601	1.603	1.608	1.612	1.620	1.630
	1.086 (CH)	1.100	1.100	1.100	1.100	1.100	1.099	1.098	1.096	1.093	1.090
H ₂ O	0.958	0.971	0.971	0.971	0.970	0.970	0.970	0.970	0.969	0.969	0.970
H ₂ S	1.336	1.354	1.354	1.353	1.353	1.353	1.353	1.352	1.352	1.355	1.363
H ₂ Si	1.514	1.538	1.538	1.538	1.537	1.537	1.534	1.528	1.522	1.514	1.511
HCCCN	1.062 (CH)	1.075	1.075	1.075	1.075	1.075	1.075	1.074	1.073	1.071	1.068
	1.206 (C≡C)	1.208	1.208	1.208	1.208	1.208	1.208	1.208	1.209	1.217	1.231
	1.376 (CC)	1.355	1.355	1.355	1.355	1.355	1.354	1.353	1.350	1.340	1.326
	1.161 (C≡N)	1.162	1.162	1.162	1.162	1.162	1.162	1.162	1.163	1.170	1.181
HCCH	1.061 (CH)	1.074	1.074	1.074	1.074	1.074	1.074	1.073	1.072	1.070	1.068
	1.203 (CC)	1.202	1.202	1.202	1.201	1.201	1.201	1.201	1.200	1.204	1.213
HCl (¹ Σ ⁺)	1.275	1.291	1.291	1.291	1.291	1.291	1.291	1.290	1.290	1.294	1.309
HCN	1.065 (CH)	1.079	1.079	1.079	1.079	1.079	1.078	1.078	1.077	1.075	1.073
	1.153 (CN)	1.151	1.151	1.151	1.151	1.151	1.150	1.150	1.150	1.151	1.158
HCP	1.066 (CH)	1.083	1.083	1.083	1.083	1.083	1.082	1.082	1.081	1.078	1.076
	1.540 (CP)	1.537	1.537	1.536	1.536	1.536	1.536	1.536	1.539	1.554	1.575
HF (¹ Σ ⁺)	0.917	0.932	0.932	0.932	0.931	0.931	0.931	0.931	0.930	0.930	0.932
HNC	0.994 (NH)	1.009	1.009	1.009	1.009	1.009	1.009	1.008	1.007	1.006	1.005
	1.169 (NC)	1.168	1.168	1.168	1.168	1.167	1.167	1.167	1.167	1.168	1.173
HOCl	0.964 (OH)	0.978	0.977	0.977	0.977	0.977	0.977	0.977	0.977	0.978	0.979
	1.689 (OCl)	1.678	1.678	1.678	1.678	1.678	1.678	1.685	1.703	1.781	1.992
LiCl (¹ Σ ⁺)	2.021	2.004	2.004	2.004	2.003	2.003	2.002	2.001	2.004	2.024	2.047
LiF (¹ Σ ⁺)	1.564	1.560	1.560	1.560	1.560	1.559	1.559	1.558	1.559	1.569	1.585
LiH (¹ Σ ⁺)	1.596	1.603	1.603	1.602	1.601	1.600	1.598	1.601	1.608	1.620	1.627
MgO (¹ Σ ⁺)	1.749	1.726	1.726	1.733	1.744	1.754	1.765	1.779	1.789	1.803	1.815
MgS (¹ Σ ⁺)	2.143	2.130	2.130	2.139	2.155	2.170	2.187	2.209	2.225	2.250	2.273
N ₂ (¹ Σ _g ⁺)	1.098	1.095	1.095	1.095	1.095	1.095	1.095	1.095	1.095	1.096	1.100
N ₂ O	1.127 (NN)	1.130	1.130	1.130	1.130	1.130	1.130	1.129	1.129	1.133	1.141
	1.185 (NO)	1.175	1.175	1.175	1.175	1.175	1.175	1.174	1.174	1.176	1.182
NaCl (¹ Σ ⁺)	2.361	2.335	2.335	2.335	2.334	2.334	2.333	2.338	2.350	2.379	2.405
NaF (¹ Σ ⁺)	1.926	1.908	1.908	1.908	1.908	1.907	1.907	1.909	1.917	1.935	1.950
NaH (¹ Σ ⁺)	1.887	1.867	1.867	1.867	1.866	1.865	1.866	1.874	1.887	1.910	1.925
NF (³ Σ ⁻)	1.317	1.302	1.302	1.302	1.302	1.302	1.301	1.301	1.301	1.308	1.334
NH (³ Σ ⁻)	1.036	1.054	1.054	1.054	1.054	1.054	1.054	1.053	1.052	1.050	1.051
NH ₃	1.012	1.007	1.007	1.007	1.007	1.007	1.007	1.006	1.006	1.006	1.007
O ₂ (³ Σ _g ⁻)	1.208	1.203	1.203	1.203	1.203	1.203	1.203	1.202	1.202	1.206	1.219
O ₃	1.272	1.250	1.250	1.250	1.250	1.251	1.253	1.260	1.269	1.285	1.298
OCS	1.147 (CO)	1.160	1.160	1.160	1.160	1.160	1.160	1.160	1.160	1.163	1.168
	1.561 (CS)	1.556	1.556	1.556	1.556	1.555	1.555	1.554	1.555	1.561	1.572
P ₂ (¹ Σ _g ⁺)	1.893	1.890	1.890	1.890	1.890	1.890	1.890	1.893	1.904	1.939	1.981
PF (³ Σ ⁻)	1.590	1.600	1.600	1.600	1.600	1.600	1.599	1.600	1.603	1.616	1.642
PH (³ Σ ⁻)	1.422	1.442	1.442	1.441	1.441	1.441	1.440	1.440	1.440	1.447	1.460
PH ₃	1.413	1.431	1.431	1.431	1.431	1.431	1.430	1.429	1.427	1.425	1.426
PN (¹ Σ ⁺)	1.491	1.486	1.486	1.486	1.486	1.486	1.486	1.486	1.488	1.500	1.520

S_2 ($^3\Sigma_g^-$)	1.889	1.896	1.896	1.896	1.895	1.895	1.895	1.898	1.909	1.951	2.016
S_2O	1.884 (SS)	1.889	1.889	1.889	1.889	1.889	1.892	1.902	1.916	1.946	1.981
	1.456 (SO)	1.463	1.463	1.463	1.463	1.463	1.463	1.467	1.473	1.484	1.497
SCS	1.553	1.551	1.551	1.551	1.551	1.550	1.550	1.550	1.552	1.558	1.568
SiO ($^1\Sigma^+$)	1.510	1.515	1.515	1.515	1.515	1.514	1.514	1.514	1.516	1.528	1.547
SiS ($^1\Sigma^+$)	1.929	1.936	1.936	1.936	1.936	1.935	1.935	1.938	1.946	1.978	2.018
SO ($^3\Sigma^-$)	1.481	1.489	1.489	1.489	1.489	1.489	1.489	1.489	1.491	1.504	1.529
SO_2	1.431	1.440	1.440	1.440	1.440	1.440	1.440	1.441	1.444	1.456	1.471
B_2H_6	1.314 (BH $\times 2$)	1.312	1.312	1.312	1.312	1.311	1.311	1.310	1.308	1.306	1.305
	1.184 (BH $\times 4$)	1.198	1.198	1.198	1.198	1.198	1.197	1.196	1.195	1.193	1.191
cyclopropane	1.501 (CC)	1.492	1.492	1.492	1.492	1.492	1.492	1.491	1.490	1.488	1.486
	1.083 (CH)	1.091	1.091	1.091	1.091	1.091	1.091	1.090	1.089	1.087	1.086
C_2^- ($^2\Sigma_g^+$)	1.268	1.258	1.258	1.259	1.262	1.265	1.269	1.273	1.275	1.277	1.283
NH^- ($^2\Pi_i$)	1.047	1.051	1.051	1.051	1.051	1.051	1.050	1.050	1.050	1.048	1.048
AlH^+ ($^2\Sigma^+$)	1.602	1.642	1.642	1.642	1.641	1.640	1.639	1.635	1.632	1.630	1.634
Cl_2^+ ($^2\Pi_{3/2g}$)	1.892	1.893	1.893	1.893	1.893	1.892	1.892	1.894	1.901	1.941	2.059
CO^+ ($^2\Sigma^+$)	1.115	1.114	1.114	1.114	1.114	1.114	1.114	1.115	1.118	1.127	1.138
HCl^+ ($^2\Pi_i$)	1.315	1.339	1.339	1.339	1.339	1.339	1.338	1.337	1.336	1.336	1.341
He_2^+ ($^2\Sigma_u^+$)	1.081	1.161	1.161	1.161	1.161	1.161	1.160	1.159	1.159	1.167	1.209
HF^+ ($^2\Pi_i$)	1.001	1.028	1.028	1.028	1.028	1.028	1.028	1.027	1.027	1.027	1.028
N_2^+ ($^2\Sigma_g^+$)	1.116	1.107	1.107	1.107	1.107	1.108	1.111	1.116	1.121	1.126	1.132
NH^+ ($^2\Pi_r$)	1.070	1.098	1.099	1.098	1.098	1.098	1.099	1.101	1.104	1.110	1.112
NH_3^+	1.014	1.037	1.037	1.037	1.037	1.037	1.036	1.036	1.035	1.035	1.035
O_2^+ ($^2\Pi_g$)	1.116	1.110	1.110	1.110	1.110	1.110	1.110	1.110	1.110	1.110	1.114
PF^+ ($^2\Pi_r$)	1.500	1.517	1.517	1.517	1.517	1.517	1.517	1.516	1.516	1.518	1.527
H_2O^+ (2B_1)	0.999	1.019	1.019	1.019	1.019	1.019	1.018	1.016	1.014	1.011	1.009
AlS ($^2\Sigma^+$)	2.029	2.031	2.031	2.032	2.040	2.052	2.069	2.089	2.103	2.129	2.154
$BeCl$ ($^2\Sigma^+$)	1.797	1.789	1.789	1.789	1.788	1.788	1.788	1.787	1.787	1.795	1.811
BeF ($^2\Sigma^+$)	1.361	1.358	1.358	1.358	1.358	1.358	1.358	1.358	1.358	1.361	1.369
BeH ($^2\Sigma^+$)	1.343	1.361	1.361	1.360	1.360	1.359	1.358	1.354	1.351	1.350	1.353
BO ($^2\Sigma^+$)	1.205	1.204	1.204	1.204	1.204	1.203	1.203	1.204	1.207	1.217	1.229
BS ($^2\Sigma^+$)	1.609	1.609	1.609	1.609	1.609	1.609	1.610	1.616	1.626	1.650	1.675
CCl ($^2\Pi_{1/2}, ^2\Pi_{3/2}$)	1.645	1.632	1.631	1.631	1.631	1.630	1.630	1.629	1.627	1.624	1.628
CF ($^2\Pi_r$)	1.272	1.263	1.262	1.262	1.262	1.262	1.262	1.262	1.262	1.262	1.263
CH ($^2\Pi_r$)	1.120	1.139	1.139	1.139	1.139	1.139	1.138	1.136	1.134	1.128	1.123
CH_3	1.076	1.089	1.089	1.089	1.089	1.089	1.088	1.088	1.087	1.086	1.086
ClO ($^2\Pi_i$)	1.570	1.553	1.552	1.552	1.552	1.552	1.551	1.551	1.553	1.564	1.592
CN ($^2\Sigma^+$)	1.172	1.166	1.166	1.166	1.167	1.168	1.171	1.176	1.180	1.185	1.191
CP ($^2\Sigma^+$)	1.562	1.555	1.555	1.555	1.557	1.562	1.570	1.581	1.590	1.609	1.630
H_2N (2B_1)	1.025	1.039	1.039	1.039	1.038	1.038	1.037	1.034	1.031	1.026	1.024
HO	0.970	0.986	0.985	0.985	0.985	0.985	0.985	0.984	0.984	0.983	0.983
HOO	0.971 (OH)	0.991	0.991	0.991	0.991	0.991	0.990	0.988	0.988	0.989	0.993
	1.331 (OO)	1.308	1.308	1.308	1.309	1.311	1.314	1.317	1.319	1.321	1.329
$MgCl$ ($^2\Sigma^+$)	2.199	2.196	2.196	2.196	2.196	2.195	2.195	2.197	2.203	2.225	2.252
MgF ($^2\Sigma^+$)	1.750	1.756	1.756	1.756	1.756	1.755	1.755	1.755	1.757	1.767	1.781
MgH ($^2\Sigma^+$)	1.730	1.753	1.753	1.752	1.752	1.750	1.748	1.743	1.740	1.742	1.748
NO ($^2\Pi_r$)	1.151	1.146	1.146	1.146	1.146	1.146	1.146	1.145	1.145	1.146	1.150
NO_2 (2A_1)	1.195	1.189	1.189	1.189	1.189	1.189	1.189	1.191	1.193	1.203	1.216
NS ($^2\Pi_r$)	1.494	1.491	1.491	1.491	1.491	1.491	1.490	1.490	1.491	1.497	1.510
OP ($^2\Pi_r$)	1.474	1.481	1.481	1.481	1.481	1.481	1.481	1.481	1.481	1.488	1.501
SF ($^2\Pi_{3/2}, ^2\Pi_{1/2}$)	1.601	1.601	1.601	1.601	1.601	1.601	1.601	1.603	1.608	1.627	1.660
SH ($^2\Pi_i$)	1.345	1.359	1.359	1.358	1.358	1.358	1.358	1.357	1.356	1.358	1.367

SiCl ($^2\Pi_r$)	2.058	2.058	2.058	2.058	2.057	2.057	2.056	2.055	2.056	2.066	2.093
SiF ($^2\Pi_r$)	1.601	1.617	1.617	1.617	1.617	1.617	1.617	1.616	1.616	1.617	1.623
SiH ($^2\Pi_r$)	1.520	1.545	1.545	1.545	1.545	1.544	1.544	1.542	1.541	1.537	1.533
SiN ($^2\Sigma^+$)	1.572	1.564	1.564	1.568	1.578	1.586	1.594	1.600	1.606	1.619	1.636
HCO	1.119 (CH)	1.138	1.138	1.138	1.137	1.137	1.135	1.129	1.122	1.112	1.106
	1.175 (CO)	1.172	1.172	1.172	1.172	1.172	1.172	1.173	1.174	1.178	1.184
MSE		0.004	0.004	0.004	0.005	0.005	0.005	0.006	0.008	0.015	0.030
MAE		0.013	0.013	0.013	0.013	0.013	0.013	0.013	0.014	0.021	0.036
rms		0.017	0.017	0.017	0.017	0.017	0.018	0.019	0.021	0.037	0.080
Max(-)		-0.091	-0.091	-0.091	-0.091	-0.091	-0.092	-0.095	-0.101	-0.110	-0.110
Max(+)		0.081	0.081	0.080	0.080	0.080	0.080	0.078	0.083	0.222	0.581

TABLE S3. Singlet-triplet energy gap ($E_T - E_S$) in kcal/mol, as a function of the acene length, calculated by spin-unrestricted KS-DFT (with LDA, BLYP, and B3LYP functionals), using the 6-31G* basis set. The experimental data are taken from Refs. [3–6], and the DMRG data are taken from Ref. [7].

n -acene	Experiment	DMRG (cc-pVDZ)	DMRG (STO-3G)	B3LYP	BLYP	LDA
2	61.0	61.0	61.5	62.65	60.44	65.19
3	43.1	44.0	45.9	41.78	40.19	43.40
4	29.3	31.9	34.7	27.70	26.74	29.06
5	19.8	23.4	26.7	17.87	17.45	19.20
6		17.5	21.0	10.93	10.81	12.16
8			14.2	5.78	2.87	3.07
10			11.6	5.57	1.31	0.53
12			10.7	7.25	1.95	1.59
14				8.58	3.27	3.50
16				8.36	3.86	4.43

TABLE S4. Singlet-triplet energy gap ($E_T - E_S$) in kcal/mol, as a function of the acene length, calculated by spin-unrestricted TAO-LDA, with various θ (in mHartree), using the 6-31G* basis set. The $\theta=0$ case corresponds to spin-unrestricted KS-LDA. The experimental data are taken from Refs. [3–6].

n -acene	Experiment	$\theta=0$	$\theta=1$	$\theta=3$	$\theta=5$	$\theta=7$	$\theta=10$	$\theta=15$	$\theta=20$	$\theta=30$	$\theta=40$
2	61.0	65.19	65.19	65.20	65.14	64.77	63.24	58.24	51.90	40.20	32.01
3	43.1	43.40	43.40	43.40	43.38	43.22	42.41	39.59	35.80	28.42	23.03
4	29.3	29.06	29.06	29.06	29.05	29.01	28.81	27.82	26.04	21.64	17.89
5	19.8	19.20	19.20	19.21	19.31	19.60	20.17	20.64	20.11	17.39	14.60
6		12.16	12.16	12.22	12.69	13.55	14.89	16.20	16.28	14.50	12.32
8		3.07	3.07	3.97	6.01	7.85	9.71	11.28	11.73	10.86	9.38
10		0.53	0.54	1.85	4.36	5.91	7.30	8.62	9.14	8.67	7.56
12		1.59	1.60	2.63	3.95	4.82	5.83	6.97	7.48	7.21	6.34
14		3.50	3.47	3.20	3.44	3.98	4.83	5.85	6.33	6.17	5.45
16		4.43	4.35	2.83	2.86	3.37	4.14	5.04	5.49	5.39	4.78
18					2.44	2.94	3.62	4.43	4.84	4.78	4.26
20					2.18	2.62	3.22	3.95	4.34	4.30	3.84
22					1.99	2.37	2.90	3.57	3.92	3.91	3.50
24					1.82	2.15	2.64	3.25	3.58	3.58	3.21
26					1.68	1.98	2.42	2.99	3.30	3.30	2.96
28					1.55	1.83	2.24	2.76	3.05	3.06	2.75
30					1.45	1.70	2.08	2.57	2.84	2.86	2.57

32	1.35	1.59	1.94	2.40	2.66	2.68	2.41
34	1.27	1.49	1.82	2.25	2.50	2.52	2.27
36	1.20	1.40	1.71	2.12	2.36	2.38	2.15
38	1.14	1.33	1.62	2.01	2.23	2.25	2.03
40	1.08	1.26	1.54	1.90	2.12	2.14	1.94
42	1.03	1.20	1.46	1.81	2.01	2.04	1.84
44	0.98	1.14	1.39	1.72	1.92	1.94	1.76
46	0.94	1.09	1.33	1.65	1.83	1.86	1.68

TABLE S5. Singlet-triplet energy gap ($E_T - E_S$) in kcal/mol, as a function of the acene length, calculated by spin-unrestricted TAO-LDA ($\theta = 7$ mHartree), using the 6-31G basis set. The experimental data are taken from Refs. [3–6].

n -acene	Experiment	TAO-LDA ($\theta = 7$ mHartree)
2	61.0	65.79
3	43.1	44.13
4	29.3	29.85
5	19.8	20.34
6		14.17
8		8.14
10		5.99
12		4.84
14		3.99
16		3.37
18		2.93
20		2.60
22		2.34
24		2.13
26		1.95
28		1.81
30		1.68
32		1.57
34		1.47
36		1.38
38		1.31
40		1.24
42		1.18
44		1.12
46		1.07
48		1.03
50		0.98
52		0.94
54		0.91
56		0.87
58		0.84
60		0.81
62		0.79
64		0.76
66		0.74
68		0.72
70		0.70
72		0.68

TABLE S6. Active orbital occupation numbers (HOMO-6, ..., HOMO-1, HOMO, LUMO, LUMO+1, ..., and LUMO+6) for the lowest singlet states of n -acenes, calculated by spin-restricted TAO-LDA ($\theta = 7$ mHartree), using the 6-31G* basis set.

n -acene	f_{H-6}	f_{H-5}	f_{H-4}	f_{H-3}	f_{H-2}	f_{H-1}	f_H	f_L	f_{L+1}	f_{L+2}	f_{L+3}	f_{L+4}	f_{L+5}	f_{L+6}
2	2.0000	2.0000	2.0000	2.0000	2.0000	2.0000	1.9998	0.0002	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
3	2.0000	2.0000	2.0000	2.0000	2.0000	2.0000	1.9957	0.0043	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
4	2.0000	2.0000	2.0000	2.0000	2.0000	2.0000	1.9719	0.0281	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
5	2.0000	2.0000	2.0000	2.0000	2.0000	1.9997	1.8997	0.1004	0.0001	0.0000	0.0000	0.0000	0.0000	0.0000
6	2.0000	2.0000	2.0000	2.0000	2.0000	1.9986	1.7587	0.2421	0.0007	0.0000	0.0000	0.0000	0.0000	0.0000
8	2.0000	2.0000	2.0000	2.0000	1.9997	1.9848	1.3529	0.6532	0.0093	0.0001	0.0000	0.0000	0.0000	0.0000
10	2.0000	2.0000	2.0000	1.9999	1.9976	1.9320	1.0195	1.0000	0.0498	0.0011	0.0000	0.0000	0.0000	0.0000
12	2.0000	2.0000	2.0000	1.9993	1.9888	1.8176	1.2184	0.8156	0.1538	0.0063	0.0002	0.0000	0.0000	0.0000
14	2.0000	2.0000	1.9997	1.9970	1.9651	1.6458	1.3511	0.6901	0.3265	0.0233	0.0014	0.0001	0.0000	0.0000
16	2.0000	1.9999	1.9989	1.9906	1.9172	1.4478	1.4346	0.6085	0.5347	0.0623	0.0051	0.0004	0.0000	0.0000
18	1.9999	1.9995	1.9967	1.9763	1.8398	1.4903	1.2595	0.7367	0.5531	0.1317	0.0148	0.0015	0.0002	0.0000
20	1.9997	1.9985	1.9915	1.9501	1.7350	1.5293	1.0992	0.9097	0.5140	0.2330	0.0347	0.0045	0.0006	0.0001
22	1.9993	1.9964	1.9817	1.9086	1.6113	1.5577	1.0489	0.9700	0.4853	0.3589	0.0692	0.0110	0.0017	0.0003
24	1.9982	1.9921	1.9649	1.8503	1.5789	1.4799	1.1581	0.8678	0.4969	0.4637	0.1214	0.0232	0.0041	0.0007
26	1.9962	1.9847	1.9392	1.7762	1.5953	1.3513	1.2435	0.7873	0.6345	0.4469	0.1918	0.0434	0.0089	0.0018
28	1.9926	1.9728	1.9033	1.6893	1.6081	1.3107	1.2323	0.7629	0.7234	0.4336	0.2779	0.0737	0.0172	0.0039
30	1.9866	1.9553	1.8565	1.6184	1.5943	1.3641	1.1263	0.8777	0.6722	0.4229	0.3753	0.1155	0.0305	0.0076
32	1.9777	1.9311	1.7994	1.6268	1.4960	1.4070	1.0339	0.9776	0.6307	0.4784	0.4142	0.1690	0.0500	0.0138
34	1.9648	1.8996	1.7335	1.6337	1.4420	1.3988	1.0632	0.9543	0.5967	0.5820	0.4070	0.2332	0.0768	0.0232
36	1.9475	1.8606	1.6609	1.6395	1.4707	1.3059	1.1362	0.8863	0.6819	0.5685	0.4009	0.3062	0.1117	0.0367
38	1.9249	1.8143	1.6444	1.5841	1.4947	1.2193	1.1983	0.8280	0.7756	0.5449	0.3957	0.3852	0.1547	0.0551
40	1.8970	1.7616	1.6485	1.5149	1.5056	1.2511	1.1400	0.8615	0.7782	0.5249	0.4675	0.3914	0.2054	0.0791
42	1.8634	1.7036	1.6521	1.5320	1.4276	1.2962	1.0683	0.9390	0.7355	0.5504	0.5079	0.3876	0.2628	0.1090
44	1.8246	1.6552	1.6417	1.5467	1.3519	1.3348	1.0084	1.0041	0.6986	0.6316	0.4933	0.3843	0.3254	0.1449
46	1.7809	1.6578	1.5774	1.5593	1.3682	1.2796	1.0702	0.9468	0.7095	0.6666	0.4806	0.3918	0.3814	0.1865