

Supporting Information

Quinoline Triradicals: A Reactivity Study

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2,4-didehydroquinolinium cation (3) UB3LYP/cc-pVTZ 1A' singlet state (Cs) dehydrocarbon atom separation: 1.30 A				2,4-didehydroquinolinium cation (3) UB3LYP/cc-pVTZ 1A' singlet state (Cs) dehydrocarbon atom separation: 1.40 A				2,4-didehydroquinolinium cation (3) UB3LYP/cc-pVTZ 1A' singlet state (Cs) dehydrocarbon atom separation: 1.50 A			
6	0.000000	0.657148	0.000000	6	0.000000	0.660463	0.000000	6	0.000000	0.662598	0.000000
6	-0.018851	-0.771396	0.000000	6	-0.013100	-0.767470	0.000000	6	-0.006203	-0.763840	0.000000
6	-1.191283	1.384490	0.000000	6	-1.200842	1.377407	0.000000	6	-1.210692	1.368488	0.000000
6	-1.199389	-1.482316	0.000000	6	-1.189021	-1.488170	0.000000	6	-1.176668	-1.495624	0.000000
6	-2.375906	0.669532	0.000000	6	-2.379126	0.654838	0.000000	6	-2.382033	0.637462	0.000000
6	-2.374378	-0.731686	0.000000	6	-2.368475	-0.747493	0.000000	6	-2.361150	-0.765932	0.000000
1	-1.183359	2.464615	0.000000	1	-1.200212	2.457503	0.000000	1	-1.218087	2.448481	0.000000
1	-1.226702	-2.562270	0.000000	1	-1.206806	-2.568375	0.000000	1	-1.184095	-2.575993	0.000000
1	-3.319394	1.195423	0.000000	1	-3.326367	1.174038	0.000000	1	-3.333346	1.149253	0.000000
1	-3.321148	-1.254066	0.000000	1	-3.311762	-1.276114	0.000000	1	-3.300393	-1.301679	0.000000
7	1.335201	-1.241867	0.000000	7	1.337328	-1.234483	0.000000	7	1.340825	-1.222313	0.000000
1	1.640539	-2.203131	0.000000	1	1.628782	-2.201543	0.000000	1	1.619957	-2.194461	0.000000
6	1.396826	0.961427	0.000000	6	1.375672	1.015707	0.000000	6	1.352198	1.069602	0.000000
6	2.749212	1.034896	0.000000	6	2.726083	1.042769	0.000000	6	2.696275	1.052967	0.000000
1	3.673346	1.591827	0.000000	1	3.650108	1.601645	0.000000	1	3.619270	1.614479	0.000000
6	2.078820	-0.145317	0.000000	6	2.116301	-0.172346	0.000000	6	2.156759	-0.196369	0.000000

E = -401.077618 au

E (CASPT2) = -400.0814348570 au

E = -401.0890829 au

E (CASPT2) = -400.0916362405 au

E = -401.0889072 au

E (CASPT2) = -400.0923629051 au

2,4-didehydroquinolinium cation (3) UB3LYP/cc-pVTZ 1A' singlet state (Cs) dehydrocarbon atom separation: 1.60 A				2,4-didehydroquinolinium cation (3) UB3LYP/cc-pVTZ 1A' singlet state (Cs) dehydrocarbon atom separation: 1.70 A				2,4-didehydroquinolinium cation (3) UB3LYP/cc-pVTZ 1A' singlet state (Cs) dehydrocarbon atom separation: 1.80 A			
6	0.000000	0.665407	0.000000	6	0.000000	0.670728	0.000000	6	0.000000	0.679766	0.000000
6	0.000952	-0.759140	0.000000	6	0.006967	-0.752278	0.000000	6	0.012849	-0.742652	0.000000
6	-1.220112	1.360478	0.000000	6	-1.227602	1.357126	0.000000	6	-1.234656	1.358023	0.000000

6	-1.164243	-1.501751	0.000000	6	-1.154666	-1.502876	0.000000	6	-1.147270	-1.498776	0.000000
6	-2.384542	0.621165	0.000000	6	-2.386513	0.611418	0.000000	6	-2.388615	0.607257	0.000000
6	-2.353639	-0.783238	0.000000	6	-2.347937	-0.793775	0.000000	6	-2.343685	-0.798752	0.000000
1	-1.235450	2.440294	0.000000	1	-1.249285	2.436713	0.000000	1	-1.261352	2.437394	0.000000
1	-1.161055	-2.582195	0.000000	1	-1.142994	-2.583334	0.000000	1	-1.127416	-2.579262	0.000000
1	-3.339706	1.125808	0.000000	1	-3.344480	1.110789	0.000000	1	-3.348830	1.102367	0.000000
1	-3.288807	-1.326017	0.000000	1	-3.279701	-1.342301	0.000000	1	-3.272587	-1.351999	0.000000
7	1.344021	-1.208172	0.000000	7	1.344916	-1.196918	0.000000	7	1.343561	-1.189635	0.000000
1	1.610051	-2.185307	0.000000	1	1.593690	-2.179631	0.000000	1	1.569612	-2.178649	0.000000
6	1.328380	1.118924	0.000000	6	1.307445	1.160084	0.000000	6	1.290007	1.195482	0.000000
6	2.662754	1.060394	0.000000	6	2.630679	1.058234	0.000000	6	2.602265	1.046017	0.000000
1	3.584039	1.624559	0.000000	1	3.551787	1.621457	0.000000	1	3.522876	1.608147	0.000000
6	2.200913	-0.222227	0.000000	6	2.247723	-0.256206	0.000000	6	2.294568	-0.298124	0.000000

E = -401.0846221 au

E (CASPT2) = -400.0894097264 au

E = -401.0802608 au

E (CASPT2) = -400.0869654784 au

E = -401.0772034 au

E (CASPT2) = -400.0863155784 au

2,4-didehydroquinolinium cation (3)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 1.90 A

6	0.000000	0.692681	0.000000
6	0.017925	-0.730701	0.000000
6	-1.240082	1.364138	0.000000
6	-1.142672	-1.488807	0.000000
6	-2.390781	0.610252	0.000000
6	-2.341583	-0.796094	0.000000
1	-1.270372	2.443311	0.000000
1	-1.117593	-2.569342	0.000000
1	-3.352295	1.102907	0.000000
1	-3.268048	-1.353282	0.000000

2,4-didehydroquinolinium cation (3)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 2.00 A

6	0.000000	0.709373	0.000000
6	0.023182	-0.716559	0.000000
6	-1.244701	1.374226	0.000000
6	-1.139695	-1.473900	0.000000
6	-2.393142	0.618406	0.000000
6	-2.340836	-0.787916	0.000000
1	-1.277684	2.453250	0.000000
1	-1.110527	-2.554551	0.000000
1	-3.355332	1.109819	0.000000
1	-3.265172	-1.348470	0.000000

2,4-didehydroquinolinium cation (3)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 2.10 A

6	-0.037949	-0.724471	0.000000
6	0.000000	0.701468	0.000000
6	1.181787	-1.437721	0.000000
6	1.198052	1.406372	0.000000
6	2.361534	-0.734410	0.000000
6	2.369008	0.673754	0.000000
1	1.167689	-2.517299	0.000000
1	1.213436	2.487542	0.000000
1	3.301727	-1.266732	0.000000
1	3.315687	1.195673	0.000000

7	1.340279	-1.189387	0.000000	7	1.335582	-1.195330	0.000000	7	-1.272465	1.269165	0.000000
1	1.538153	-2.185069	0.000000	1	1.499480	-2.197734	0.000000	1	-1.360210	2.281204	0.000000
6	1.277132	1.226547	0.000000	6	1.268286	1.254974	0.000000	6	-1.316519	-1.251027	0.000000
6	2.579299	1.022661	0.000000	6	2.560547	0.990796	0.000000	6	-2.582396	-0.820225	0.000000
1	3.501870	1.579384	0.000000	1	3.486712	1.539684	0.000000	1	-3.531304	-1.328533	0.000000
6	2.338484	-0.349377	0.000000	6	2.378601	-0.408516	0.000000	6	-2.373479	0.563591	0.000000

E = -401.0751416 au

E (CASPT2) = -400.0868896427 au

E = -401.0730522 au

E (CASPT2) = -400.0873813133 au

E = -401.0719064 au

E (CASPT2) = -400.0876309454 au

2,4-didehydroquinolinium cation (3)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 2.20 A

6	-0.053117	-0.742890	0.000000
6	0.000000	0.685422	0.000000
6	1.162101	-1.465408	0.000000
6	1.210947	1.371889	0.000000
6	2.350483	-0.778498	0.000000
6	2.374106	0.629585	0.000000
1	1.135005	-2.544862	0.000000
1	1.238490	2.453058	0.000000
1	3.284000	-1.322479	0.000000
1	3.325851	1.142142	0.000000
7	-1.247035	1.306698	0.000000
1	-1.282133	2.322089	0.000000
6	-1.330805	-1.278690	0.000000
6	-2.572010	-0.737363	0.000000
1	-3.531821	-1.225527	0.000000
6	-2.381728	0.654069	0.000000

2,4-didehydroquinolinium cation (3)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 2.30 A

6	-0.069089	-0.762381	0.000000
6	0.000000	0.669931	0.000000
6	1.140522	-1.494829	0.000000
6	1.224788	1.334996	0.000000
6	2.338318	-0.825630	0.000000
6	2.379536	0.581700	0.000000
1	1.099517	-2.573969	0.000000
1	1.266354	2.415967	0.000000
1	3.264286	-1.382395	0.000000
1	3.336695	1.083998	0.000000
7	-1.219580	1.347750	0.000000
1	-1.197900	2.363713	0.000000
6	-1.348989	-1.301576	0.000000
6	-2.561619	-0.656919	0.000000
1	-3.534311	-1.120376	0.000000
6	-2.386397	0.751174	0.000000

2-dehydroquinolinium cation (1)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

6	2.381298	0.666689	0.000000
6	1.213828	1.396151	0.000000
6	0.000000	0.705617	0.000000
6	-0.052611	-0.716252	0.000000
6	1.172682	-1.423847	0.000000
6	2.362343	-0.742701	0.000000
1	-1.217214	2.391771	0.000000
1	3.329961	1.185013	0.000000
1	1.231828	2.477738	0.000000
6	-1.309283	-1.358707	0.000000
1	1.152852	-2.504833	0.000000
1	3.296848	-1.284952	0.000000
6	-2.495508	-0.641515	0.000000
6	-2.350464	0.723804	0.000000
1	-1.345846	-2.441337	0.000000
1	-3.466274	-1.112495	0.000000
7	-1.216552	1.376237	0.000000

E = -401.0705578 au
E (CASPT2) = -400.0850155601 au

E = -401.0665369 au
E (CASPT2) = -400.0792351060 au

E = -401.749559 au
S2 = 0.757307
ZPVE = 0.135966 au
(H298 - E0) = 0.007736 au
E (CASPT2) = -400.7436087589 au

4-dehydroquinolinium cation (2)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

6	-2.386413	0.687690	0.000000
6	-1.193323	1.370621	0.000000
6	0.000000	0.638064	0.000000
6	-0.021257	-0.792145	0.000000
6	-1.269848	-1.457266	0.000000
6	-2.426591	-0.723458	0.000000
1	1.237339	2.270351	0.000000
1	-3.313890	1.242909	0.000000
1	-1.171818	2.452554	0.000000
6	1.229315	-1.392229	0.000000
1	-1.286282	-2.537211	0.000000
1	-3.383792	-1.224680	0.000000
6	2.441800	-0.774417	0.000000
6	2.400551	0.618976	0.000000
1	3.387302	-1.296785	0.000000
1	3.289223	1.233875	0.000000
7	1.228074	1.257710	0.000000

E = -401.754311 au
S2 = 0.757429
ZPVE = 0.136477 au
(H298 - E0) = 0.007705 au

2,4-didehydroquinolinium cation (3)

UB3LYP/cc-pVTZ

3A' triplet state (Cs)

6	-2.381213	0.533553	0.000000
6	-1.241044	1.304153	0.000000
6	0.000000	0.660841	0.000000
6	0.087307	-0.765967	0.000000
6	-1.108526	-1.520684	0.000000
6	-2.317559	-0.875157	0.000000
1	1.138930	2.398403	0.000000
1	-3.346751	1.019609	0.000000
1	-1.297256	2.384664	0.000000
6	1.379653	-1.285107	0.000000
1	-1.044147	-2.598753	0.000000
1	-3.234876	-1.445809	0.000000
6	2.547518	-0.575554	0.000000
6	2.355810	0.786468	0.000000
1	3.533485	-1.022383	0.000000
7	1.188420	1.384142	0.000000

E = -401.050853 au
S2 = 2.019117
ZPVE = 0.122870 au
(H298 - E0) = 0.007756 au
E (CASPT2) = -400.0505066712 au

2,4-didehydroquinolinium cation (2)

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

6	-2.365252	-0.755634	0.000000
6	-1.183662	-1.491761	0.000000
6	-0.010069	-0.766258	0.000000
6	0.000000	0.661045	0.000000
6	-1.205153	1.373487	0.000000
6	-2.380398	0.647176	0.000000
1	1.625742	-2.198528	0.000000
1	-3.306801	-1.287349	0.000000
1	-1.197139	-2.572015	0.000000
6	1.365454	1.039350	0.000000
1	-1.208022	2.453523	0.000000
1	-3.329449	1.163114	0.000000
6	2.713806	1.047796	0.000000
6	2.132793	-0.181922	0.000000
1	3.637859	1.607202	0.000000
7	1.338956	-1.229374	0.000000

E = -401.0899025 au
S2 = 0
ZPVE = 0.123274 au
(H298 - E0) = 0.007650 au
E (CASPT2) = -400.0928115351 au

E (CASPT2) = -400.7477611147 au

2,4,5-tridehydroquinolinium cation (4)
UB3LYP/cc-pVTZ
4A' quartet state (Cs)

6	2.394137	0.537756	0.000000
6	1.234001	1.283451	0.000000
6	0.000000	0.626544	0.000000
6	-0.067429	-0.809599	0.000000
6	1.157073	-1.473000	0.000000
6	2.371674	-0.880681	0.000000
1	-1.184725	2.335408	0.000000
1	3.349639	1.045077	0.000000
1	1.275630	2.364496	0.000000
6	-1.342614	-1.366127	0.000000
1	3.295473	-1.443012	0.000000
6	-2.522109	-0.675905	0.000000
6	-2.357289	0.690721	0.000000
1	-3.499980	-1.140530	0.000000
7	-1.205814	1.319943	0.000000

E = -400.3548514 au

S2 = 3.785359

ZPVE = 0.109740 au

(H298 - E0) = 0.007737 au

E (CASPT2) = -399.3590474353 au

2,4,5-tridehydroquinolinium cation (4)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

6	2.398623	-0.695464	0.000000
6	1.216405	-1.433623	0.000000
6	0.031345	-0.726327	0.000000
6	0.000000	0.709552	0.000000
6	1.218776	1.360003	0.000000
6	2.417048	0.715105	0.000000
1	-1.593187	-2.171510	0.000000
1	3.343049	-1.223418	0.000000
1	1.240501	-2.513673	0.000000
6	-1.367309	1.071733	0.000000
1	3.358611	1.246836	0.000000
6	-2.715732	1.064471	0.000000
6	-2.116446	-0.157704	0.000000
1	-3.645731	1.613985	0.000000
7	-1.314214	-1.199815	0.000000

E = -400.3942693 au

S2 = 0.758452

ZPVE = 0.110194 au

(H298 - E0) = 0.007617 au

E (CASPT2) = -399.4011458770 au

2,4,6-tridehydroquinolinium cation (5)
UB3LYP/cc-pVTZ
4A' quartet state (Cs)

6	-2.390759	0.744455	0.000000
6	-1.173438	1.398702	0.000000
6	0.000000	0.633150	0.000000
6	-0.034020	-0.799321	0.000000
6	-1.296088	-1.451080	0.000000
6	-2.379619	-0.643331	0.000000
1	1.289452	2.262269	0.000000
1	-3.316641	1.304261	0.000000
1	-1.122702	2.480229	0.000000
6	1.210389	-1.428826	0.000000
1	-1.350082	-2.531151	0.000000
6	2.433489	-0.822224	0.000000
6	2.359898	0.552337	0.000000
1	3.377163	-1.353060	0.000000
7	1.249098	1.247755	0.000000

E = -400.3558012 au

S2 = 3.769915

ZPVE = 0.109601 au

(H298 - E0) = 0.007745 au

E (CASPT2) = -399.3601113424 au

2,4,6-tridehydroquinolinium cation (5)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

6	-2.481739	-0.568315	0.000000
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2,4,7-tridehydroquinolinium cation (6)
UB3LYP/cc-pVTZ
4A' quartet state (Cs)

6	-2.329591	0.687693	0.000000
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2,4,7-tridehydroquinolinium cation (6)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

6	-2.411617	-0.521679	0.000000
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6	-1.344319	-1.381265	0.000000	6	-1.193772	1.431068	0.000000	6	-1.370081	-1.413529	0.000000
6	-0.122813	-0.733354	0.000000	6	0.000000	0.692381	0.000000	6	-0.131938	-0.789278	0.000000
6	0.000000	0.691853	0.000000	6	-0.026805	-0.741302	0.000000	6	0.000000	0.636450	0.000000
6	-1.152506	1.500366	0.000000	6	-1.272928	-1.416804	0.000000	6	-1.132079	1.464910	0.000000
6	-2.322324	0.803663	0.000000	6	-2.445365	-0.695028	0.000000	6	-2.380152	0.859063	0.000000
1	1.398111	-2.287445	0.000000	1	1.276085	2.330938	0.000000	1	1.374575	-2.356452	0.000000
1	-3.466706	-1.016688	0.000000	1	-1.195576	2.514242	0.000000	1	-1.504380	-2.486702	0.000000
1	-1.428985	-2.458861	0.000000	6	1.220170	-1.357925	0.000000	6	1.392048	0.892940	0.000000
6	1.391640	0.961879	0.000000	1	-1.280728	-2.497702	0.000000	1	-1.029194	2.540856	0.000000
1	-1.094574	2.579980	0.000000	1	-3.408380	-1.186647	0.000000	1	-3.287303	1.447068	0.000000
6	2.736183	0.863293	0.000000	6	2.442197	-0.744736	0.000000	6	2.737280	0.785366	0.000000
6	2.059510	-0.316896	0.000000	6	2.360204	0.627279	0.000000	6	2.052160	-0.388630	0.000000
1	3.701350	1.348469	0.000000	1	3.388495	-1.270605	0.000000	1	3.705552	1.264043	0.000000
7	1.187001	-1.298972	0.000000	7	1.242207	1.316289	0.000000	7	1.172431	-1.366070	0.000000

E = -400.3953109 au
S2 = 0.756967
ZPVE = 0.109987 au
(H298 - E0) = 0.007640 au
E (CASPT2) = -399.4026052580 au

E = -400.3565046 au
S2 = 3.778833
ZPVE = 0.109553 au
(H298 - E0) = 0.007753 au
E (CASPT2) = -399.3607806199 au

E = -400.3970571 au
S2 = 0.757571
ZPVE = 0.109995 au
(H298 - E0) = 0.007624 au
E (CASPT2) = -399.4043220564 au

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

4A' quartet state (Cs)

6	2.415757	0.605360	0.000000
6	1.248834	1.292163	0.000000
6	0.000000	0.700230	0.000000
6	-0.064941	-0.730984	0.000000
6	1.143598	-1.465954	0.000000
6	2.351377	-0.813915	0.000000
1	-1.136629	2.435750	0.000000

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

6	2.424439	-0.746916	0.000000
6	1.243230	-1.438076	0.000000
6	0.033843	-0.811894	0.000000
6	0.000000	0.623339	0.000000
6	1.194036	1.355332	0.000000
6	2.392103	0.664587	0.000000
1	-1.555728	-2.287830	0.000000

quinoline

RB3LYP/cc-pVTZ

1A' singlet state (Cs)

6	0.000000	0.703083	0.000000
6	-0.043632	-0.722995	0.000000
6	-1.316836	-1.335670	0.000000
6	1.169908	-1.450819	0.000000
6	-2.438148	-0.551852	0.000000
6	2.373301	-0.795499	0.000000
6	-2.285788	0.852703	0.000000

1	3.374851	1.107346	0.000000	1	3.376002	-1.263394	0.000000	6	2.416346	0.616251	0.000000
6	-1.355079	-1.263636	0.000000	6	-1.376405	0.962373	0.000000	7	-1.127025	1.466934	0.000000
1	1.094669	-2.545087	0.000000	1	1.173921	2.435205	0.000000	6	1.258627	1.349546	0.000000
1	3.274080	-1.377243	0.000000	1	3.327516	1.205816	0.000000	1	-1.389190	-2.416339	0.000000
6	-2.524406	-0.557795	0.000000	6	-2.725835	0.936652	0.000000	1	1.132217	-2.533169	0.000000
6	-2.346330	0.808436	0.000000	6	-2.113270	-0.277921	0.000000	1	-3.428969	-0.984769	0.000000
1	-3.508221	-1.010102	0.000000	1	-3.662898	1.474149	0.000000	1	3.297216	-1.358122	0.000000
7	-1.187372	1.420843	0.000000	7	-1.298809	-1.309830	0.000000	1	-3.167433	1.485952	0.000000
								1	3.374407	1.118880	0.000000
								1	1.268250	2.430534	0.000000

E = -400.3537627 au
S2 = 3.772836
ZPVE = 0.109895 au
(H298 - E0) = 0.007738 au
E (CASPT2) = -399.3578259361 au

E = -400.3944382 au
S2 = 0.75737
ZPVE = 0.110229 au
(H298 - E0) = 0.007624 au
E (CASPT2) = -399.4009184152 au

E = -402.0675817 au
ZPVE = 0.135471 au
(H298 - E0) = 0.007591 au
E (CASPT2) = -401.0630288899 au

quinolinium cation				2-dehydroquinoline				4-dehydroquinoline			
RB3LYP/cc-pVTZ				UB3LYP/cc-pVTZ				UB3LYP/cc-pVTZ			
1A' singlet state (Cs)				2A' doublet state (Cs)				2A' doublet state (Cs)			
6	0.000000	0.677047	0.000000	6	2.271257	-0.947075	0.000000	6	-2.414213	0.498551	0.000000
6	0.041796	-0.745606	0.000000	6	1.027911	-1.530549	0.000000	6	-1.280752	1.268888	0.000000
6	-1.176608	-1.450853	0.000000	6	-0.125371	-0.724062	0.000000	6	0.000000	0.668501	0.000000
6	1.308271	-1.377079	0.000000	6	0.000000	0.694970	0.000000	6	0.079274	-0.769807	0.000000
6	-2.385260	-0.784559	0.000000	6	1.295034	1.260447	0.000000	6	-1.110673	-1.534351	0.000000
6	2.452930	-0.624603	0.000000	6	2.406830	0.455736	0.000000	6	-2.330553	-0.910630	0.000000
6	-2.387477	0.603045	0.000000	1	3.157515	-1.567448	0.000000	1	-3.386653	0.972535	0.000000
6	2.385013	0.785115	0.000000	1	0.901890	-2.604138	0.000000	1	-1.326396	2.349033	0.000000
7	-1.235649	1.275276	0.000000	6	-1.188743	1.472066	0.000000	6	1.378209	-1.271257	0.000000
6	1.176086	1.438519	0.000000	1	1.397272	2.338397	0.000000	1	-1.036381	-2.613041	0.000000
1	-1.267745	2.287396	0.000000	1	3.394381	0.896709	0.000000	1	-3.238061	-1.499026	0.000000
1	-1.156467	-2.532764	0.000000	6	-2.416412	0.863910	0.000000	6	2.495971	-0.517328	0.000000

1	1.354762	-2.457143	0.000000	6	-2.396634	-0.546957	0.000000	6	2.283920	0.892698	0.000000
1	-3.324786	-1.314672	0.000000	1	-1.110017	2.553234	0.000000	1	3.499965	-0.919068	0.000000
1	3.419089	-1.108177	0.000000	1	-3.339695	1.423214	0.000000	1	3.146903	1.552144	0.000000
1	-3.292081	1.192463	0.000000	7	-1.377797	-1.290128	0.000000	7	1.104789	1.457976	0.000000
1	3.299980	1.360509	0.000000								
1	1.128282	2.519298	0.000000								

E = -402.4481634 au
ZPVE = 0.149625 au
(H298 - E0) = 0.007731 au
E (CASPT2) = -401.4389213341 au

E = -401.389748 au
S2 = 0.754922
ZPVE = 0.122683 au
(H298 - E0) = 0.007584 au
E (CASPT2) = -400.3866898419 au

E = -401.3795822 au
S2 = 0.757503
ZPVE = 0.122418 au
(H298 - E0) = 0.007568 au
E (CASPT2) = -400.3775278480 au

2,4-didehydroquinoline
UB3LYP/cc-pVTZ
3A' triplet state (Cs)

6	-2.392915	0.407191	0.000000
6	-1.298334	1.235920	0.000000
6	0.000000	0.690827	0.000000
6	0.158125	-0.731434	0.000000
6	-0.987398	-1.557307	0.000000
6	-2.238461	-0.994320	0.000000
1	-3.387825	0.831824	0.000000
1	-1.397301	2.312769	0.000000
6	1.491833	-1.167281	0.000000
1	-0.858446	-2.631034	0.000000
1	-3.115324	-1.627264	0.000000
6	2.579911	-0.361077	0.000000
6	2.261592	1.015201	0.000000
1	3.597411	-0.726944	0.000000
7	1.102195	1.516333	0.000000

2,4-didehydroquinoline
UB3LYP/cc-pVTZ
1A' singlet state (Cs)

6	-2.221577	1.024898	0.000000
6	-0.961293	1.581962	0.000000
6	0.151368	0.734902	0.000000
6	0.000000	-0.705151	0.000000
6	-1.316539	-1.217999	0.000000
6	-2.399284	-0.369370	0.000000
1	-3.089334	1.670807	0.000000
1	-0.812518	2.651812	0.000000
6	1.158516	-1.490632	0.000000
1	-1.454071	-2.289298	0.000000
1	-3.400781	-0.777183	0.000000
6	2.452014	-1.118775	0.000000
6	2.334864	0.285794	0.000000
1	3.365095	-1.687599	0.000000
7	1.457600	1.153953	0.000000

2,4,5-tridehydroquinolinium cation plus electron
UB3LYP/cc-pVTZ
1A' singlet state (Cs)

6	2.416211	-0.544278	0.000000
6	1.288506	-1.391244	0.000000
6	0.086349	-0.743453	0.000000
6	0.000000	0.699467	0.000000
6	1.102442	1.584783	0.000000
6	2.316068	0.843165	0.000000
1	-1.466544	-2.276992	0.000000
1	3.397030	-1.009259	0.000000
1	1.383454	-2.468083	0.000000
6	-1.391164	0.966212	0.000000
1	3.255087	1.390805	0.000000
6	-2.738431	0.897745	0.000000
6	-2.110075	-0.308276	0.000000
1	-3.696849	1.392831	0.000000
7	-1.241660	-1.293432	0.000000

E = -400.6941753 au
S2 = 2.015443
ZPVE = 0.109779 au
(H298 - E0) = 0.007600 au
E (CASPT2) = -399.6956632124 au

2,4,7-tridehydroquinolinium cation plus electron

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

6	-2.523860	-0.718661	0.000000
6	-1.299299	-1.443213	0.000000
6	-0.106094	-0.776401	0.000000
6	0.000000	0.659304	0.000000
6	-1.196410	1.409374	0.000000
6	-2.382595	0.712140	0.000000
1	1.478389	-2.271577	0.000000
1	-1.308453	-2.531816	0.000000
6	1.350946	0.981301	0.000000
1	-1.155907	2.492869	0.000000
1	-3.294531	1.303431	0.000000
6	2.705529	0.910506	0.000000
6	2.102300	-0.299220	0.000000
1	3.650906	1.429246	0.000000
7	1.246642	-1.290419	0.000000

E = -400.5954819 au
S2 = 0
ZPVE = 0.107583 au
(H298 - E0) = 0.008060 au

E = -400.7214844 au
S2 = 0
ZPVE = 0.109315 au
(H298 - E0) = 0.007646 au
E (CASPT2) = -399.7378565842 au

2,4,8-tridehydroquinolinium cation plus electron

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

6	2.353476	-0.773393	0.000000
6	1.201610	-1.583794	0.000000
6	0.092659	-0.786490	0.000000
6	0.000000	0.650910	0.000000
6	1.202473	1.380929	0.000000
6	2.367713	0.643792	0.000000
1	-1.492662	-2.258024	0.000000
1	3.330920	-1.251695	0.000000
6	-1.349946	1.010159	0.000000
1	1.202957	2.461213	0.000000
1	3.319306	1.162802	0.000000
6	-2.691395	0.955187	0.000000
6	-2.132628	-0.283973	0.000000
1	-3.628131	1.490777	0.000000
7	-1.285165	-1.269290	0.000000

E = -400.6158329 au
S2 = 0
ZPVE = 0.108182 au
(H298 - E0) = 0.007900 au

E = -400.6029402 au
S2 = 0
ZPVE = 0.108092 au
(H298 - E0) = 0.007842 au
E (CASPT2) = -399.6102917351 au

2,4,5-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

6	2.400611	0.529825	0.000000
6	1.261830	1.303681	0.000000
6	0.000000	0.693618	0.000000
6	-0.132198	-0.761106	0.000000
6	1.085073	-1.436561	0.000000
6	2.321833	-0.882314	0.000000
1	3.373751	1.003421	0.000000
1	1.315001	2.382369	0.000000
6	-1.424255	-1.294432	0.000000
1	3.221665	-1.482637	0.000000
6	-2.597731	-0.643341	0.000000
6	-2.250681	0.740721	0.000000
1	-3.606029	-1.017928	0.000000
7	-1.184469	1.373462	0.000000

E = -400.0311877 au
S2 = 1.038521
ZPVE = 0.095992 au
(H298 - E0) = 0.007669 au
E (CASPT2) = -399.0516410606 au

E (CASPT2) = -399.6027348266 au

2,4,6-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

6	-2.406064	0.702832	0.000000
6	-1.216493	1.408640	0.000000
6	0.000000	0.711000	0.000000
6	0.042248	-0.736867	0.000000
6	-1.200701	-1.431584	0.000000
6	-2.327975	-0.680755	0.000000
1	-3.356030	1.220050	0.000000
1	-1.202036	2.489351	0.000000
6	1.296092	-1.349834	0.000000
1	-1.208950	-2.512072	0.000000
6	2.512262	-0.780864	0.000000
6	2.248625	0.621222	0.000000
1	3.494972	-1.218252	0.000000
7	1.226299	1.319741	0.000000

E = -400.0316401 au

S2 = 1.029509

ZPVE = 0.095959 au

(H298 - E0) = 0.007655 au

E (CASPT2) = -399.0518974510 au

protonated dimethyl disulfide
RB3LYP/cc-pVTZ
1A singlet state (C1)

6	-2.133879	-0.379156	-0.531192
1	-1.897973	-0.426765	-1.590632

E (CASPT2) = -399.6232393252 au

2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

6	-2.296160	-0.804709	0.000000
6	-1.144878	-1.521153	0.000000
6	0.044419	-0.764796	0.000000
6	0.000000	0.683124	0.000000
6	-1.264258	1.318134	0.000000
6	-2.428147	0.574759	0.000000
1	-1.099258	-2.601306	0.000000
6	1.222138	1.362686	0.000000
1	-1.303881	2.398420	0.000000
1	-3.396000	1.056847	0.000000
6	2.469448	0.860305	0.000000
6	2.277024	-0.547168	0.000000
1	3.425401	1.353389	0.000000
7	1.299460	-1.310635	0.000000

E = -400.0326673 au

S2 = 1.032366

ZPVE = 0.095926 au

(H298 - E0) = 0.007658 au

E (CASPT2) = -399.0528969534 au

dimethyl disulfide radical cation
UB3LYP/cc-pVTZ
2A2 doublet state (C2v)

6	0.000000	1.598162	1.063730
1	-0.901442	1.272823	1.577036

2,4,8-tridehydroquinoline
UB3LYP/cc-pVTZ

2A' doublet state (Cs)

6	2.283801	-0.997319	0.000000
6	1.029224	-1.511261	0.000000
6	-0.141307	-0.780560	0.000000
6	0.000000	0.678436	0.000000
6	1.305079	1.221385	0.000000
6	2.415644	0.411414	0.000000
1	3.161718	-1.630226	0.000000
6	-1.184792	1.411929	0.000000
1	1.412651	2.295846	0.000000
1	3.405224	0.848210	0.000000
6	-2.454961	0.973005	0.000000
6	-2.362931	-0.449796	0.000000
1	-3.379848	1.522442	0.000000
7	-1.419755	-1.254239	0.000000

E = -400.0322649 au

S2 = 1.061414

ZPVE = 0.096171 au

(H298 - E0) = 0.007623 au

E (CASPT2) = -399.0495208914 au

2,5-didehydroquinoline
UBLYP/cc-pVDZ
3A' triplet state (Cs)

6	2.441403	0.552727	0.000000
6	1.283767	1.327627	0.000000

1	-2.181712	-1.368482	-0.087646	1	0.901442	1.272823	1.577036	6	0.000000	0.710233	0.000000
1	-3.053294	0.181343	-0.366658	1	0.000000	2.683220	0.964885	6	-0.104159	-0.746142	0.000000
6	2.121640	0.438923	-0.482516	6	0.000000	-1.598162	1.063730	6	1.118279	-1.444983	0.000000
1	3.015783	-0.186256	-0.488410	1	0.000000	-2.683220	0.964885	6	2.371066	-0.881290	0.000000
1	1.853897	0.692121	-1.503172	1	0.901442	-1.272823	1.577036	1	3.429234	1.037300	0.000000
1	2.299934	1.315680	0.131317	1	-0.901442	-1.272823	1.577036	1	1.326223	2.424684	0.000000
16	-0.797445	0.595359	0.246078	16	0.000000	1.012276	-0.656333	6	-1.409634	-1.339940	0.000000
16	0.874598	-0.661166	0.282154	16	0.000000	-1.012276	-0.656333	1	3.291913	-1.482202	0.000000
1	-1.197658	0.486659	1.535749					6	-2.541461	-0.530303	0.000000

E = -876.6327228 au
ZPVE = 0.086908 au
(H298 - E0) = 0.007793 au

E = -876.0191614 au
ZPVE = 0.076883 au
(H298 - E0) = 0.007511 au

6	-2.303174	0.875332	0.000000
1	-1.494023	-2.437193	0.000000
1	-3.556584	-0.947864	0.000000
7	-1.161898	1.466530	0.000000

2,5-didehydroquinoline
UBLYP/cc-pVDZ
1A' singlet state (Cs)

6	2.439220	0.610032	0.000000
6	1.261990	1.356247	0.000000
6	0.000000	0.701761	0.000000
6	-0.087912	-0.756591	0.000000
6	1.152232	-1.423291	0.000000
6	2.389966	-0.822458	0.000000
1	3.415750	1.117615	0.000000
1	1.275554	2.453607	0.000000
6	-1.393334	-1.358308	0.000000
1	3.322319	-1.406460	0.000000
6	-2.542749	-0.576846	0.000000
6	-2.326828	0.836041	0.000000
1	-1.464182	-2.454829	0.000000
1	-3.548823	-1.014589	0.000000

2,6-didehydroquinoline
UBLYP/cc-pVDZ
3A' triplet state (Cs)

6	0.000000	0.716419	0.000000
6	-0.015750	-0.732007	0.000000
6	-1.286417	-1.397302	0.000000
6	1.242235	-1.431978	0.000000
6	-2.465962	-0.659465	0.000000
6	2.383206	-0.668469	0.000000
6	-2.313052	0.759765	0.000000
6	2.448434	0.734955	0.000000
7	-1.206981	1.406982	0.000000
6	1.232993	1.431068	0.000000
1	-1.312972	-2.498529	0.000000
1	1.256821	-2.532527	0.000000
1	-3.453583	-1.138963	0.000000
1	3.407001	1.273618	0.000000
1	1.197477	2.529619	0.000000

E = -400.4394108 au
S2 = 2.010171
ZPVE = 0.105998 au
(H298 - E0) = 0.007833 au

2,6-didehydroquinoline
UBLYP/cc-pVDZ
1A' singlet state (Cs)

6	0.000000	0.716981	0.000000
6	-0.016690	-0.730938	0.000000
6	-1.287151	-1.395386	0.000000
6	1.241594	-1.432791	0.000000
6	-2.466727	-0.656423	0.000000
6	2.384416	-0.672451	0.000000
6	-2.313388	0.762112	0.000000
6	2.449243	0.730986	0.000000
7	-1.206802	1.409049	0.000000

7 -1.193731 1.415019 0.000000

E = -400.442455 au
S2 = 0.876729
ZPVE = 0.105722 au
(H298 - E0) = 0.007869 au

2,7-didehydroquinoline
UBLYP/cc-pVDZ
3A' triplet state (Cs)

6	-0.019392	-0.770370	0.000000
6	0.000000	0.678584	0.000000
6	-1.260701	1.363841	0.000000
6	1.257211	1.359901	0.000000
6	-2.455334	0.650446	0.000000
6	2.461519	0.646166	0.000000
6	-2.329787	-0.770762	0.000000
6	2.371673	-0.756118	0.000000
7	-1.233451	-1.437027	0.000000
6	1.217102	-1.499662	0.000000
1	-1.268185	2.465418	0.000000
1	1.269469	2.460833	0.000000
1	-3.433209	1.148963	0.000000
1	3.428051	1.169832	0.000000
1	1.184287	-2.598014	0.000000

E = -400.4390639 au
S2 = 2.009173
ZPVE = 0.105791 au
(H298 - E0) = 0.007841 au

E = -400.4384551 au
S2 = 2.006619
ZPVE = 0.105773 au
(H298 - E0) = 0.007850 au

2,7-didehydroquinoline
UBLYP/cc-pVDZ
1A' singlet state (Cs)

6	-0.015601	-0.771181	0.000000
6	0.000000	0.678138	0.000000
6	-1.258392	1.365925	0.000000
6	1.254625	1.364437	0.000000
6	-2.453079	0.652814	0.000000
6	2.457129	0.647980	0.000000
6	-2.320268	-0.765691	0.000000
6	2.367268	-0.753752	0.000000
7	-1.236248	-1.450220	0.000000
6	1.215178	-1.502001	0.000000
1	-1.264030	2.467814	0.000000
1	1.263928	2.465973	0.000000
1	-3.432189	1.148525	0.000000
1	3.424722	1.170108	0.000000
1	1.180145	-2.600894	0.000000

E = -400.4401179 au
S2 = 0.960388
ZPVE = 0.105498 au
(H298 - E0) = 0.007854 au

4,5-didehydroquinoline

6	1.234420	1.428839	0.000000
1	-1.315786	-2.496467	0.000000
1	1.253126	-2.533187	0.000000
1	-3.454087	-1.136513	0.000000
1	3.407628	1.269942	0.000000
1	1.202430	2.527314	0.000000

E = -400.4386441 au
S2 = 1.006176
ZPVE = 0.105735 au
(H298 - E0) = 0.007846 au

2,8-didehydroquinoline
UBLYP/cc-pVDZ
3A' triplet state (Cs)

6	-0.114942	-0.789736	0.000000
6	0.000000	0.663323	0.000000
6	-1.216787	1.423808	0.000000
6	1.301635	1.255749	0.000000
6	-2.451069	0.782361	0.000000
6	2.450889	0.470707	0.000000
6	-2.413767	-0.644452	0.000000
6	2.353011	-0.961389	0.000000
7	-1.366769	-1.384984	0.000000
6	1.095822	-1.514242	0.000000
1	-1.156045	2.524417	0.000000
1	1.382641	2.352701	0.000000
1	-3.397256	1.339114	0.000000
1	3.445434	0.940379	0.000000
1	3.263868	-1.578498	0.000000

2,8-didehydroquinoline				UBLYP/cc-pVDZ				E = -400.4352423 au						
UBLYP/cc-pVDZ				3A' triplet state (Cs)				S2 = 2.007684						
1A' singlet state (Cs)				6	0.000000	0.650931	0.000000	ZPVE = 0.105875 au						
6	-0.097280	-0.804357	0.000000	6	-0.059212	-0.827902	0.000000	(H298 - E0) = 0.007860 au						
6	0.000000	0.652527	0.000000	6	-1.353736	-1.378556	0.000000	4,5-didehydroquinoline						
6	-1.218873	1.410051	0.000000	6	1.172041	-1.510098	0.000000	UBLYP/cc-pVDZ						
6	1.296744	1.255101	0.000000	6	-2.500400	-0.629871	0.000000	1A' singlet state (Cs)						
6	-2.460549	0.785866	0.000000	6	2.412376	-0.921829	0.000000	6	0.000000	0.622924	0.000000			
6	2.452081	0.478195	0.000000	6	-2.317236	0.802156	0.000000	6	-0.063982	-0.876544	0.000000			
6	-2.417988	-0.641335	0.000000	6	2.455967	0.514646	0.000000	6	-1.379117	-1.379775	0.000000			
6	2.360668	-0.952371	0.000000	7	-1.137285	1.413293	0.000000	6	1.192977	-1.504199	0.000000			
7	-1.378019	-1.374170	0.000000	6	1.288406	1.271797	0.000000	6	-2.508258	-0.608707	0.000000			
6	1.104306	-1.514120	0.000000	1	-3.515157	-1.052523	0.000000	6	2.423584	-0.898908	0.000000			
1	-1.152863	2.509253	0.000000	1	3.344842	-1.504789	0.000000	6	-2.317492	0.820471	0.000000			
1	1.368530	2.352363	0.000000	1	-3.210767	1.450953	0.000000	6	2.461381	0.534550	0.000000			
1	-3.402874	1.347673	0.000000	1	3.435497	1.016002	0.000000	7	-1.125427	1.395712	0.000000			
1	3.442777	0.956195	0.000000	1	1.317350	2.369657	0.000000	6	1.279776	1.262712	0.000000			
1	3.275909	-1.563635	0.000000					1	-3.526963	-1.022074	0.000000			
E = -400.4385262 au				E = -400.4287742 au				1				3.357057	-1.480818	0.000000
S2 = 0.881265				S2 = 2.013638				1				-3.197512	1.485969	0.000000
ZPVE = 0.105411 au				ZPVE = 0.105615 au				1				3.432254	1.051559	0.000000
(H298 - E0) = 0.007884 au				(H298 - E0) = 0.007826 au				1				1.279934	2.360236	0.000000
4,6-didehydroquinoline				UBLYP/cc-pVDZ				E = -400.4333767 au						
UBLYP/cc-pVDZ				1A' singlet state (Cs)				S2 = 0.820762						
3A' triplet state (Cs)				6	0.000000	0.653163	0.000000	ZPVE = 0.105114 au						
6	0.000000	0.651327	0.000000	6	-0.027179	-0.814505	0.000000	(H298 - E0) = 0.007873 au						
6	-0.033247	-0.817635	0.000000	6	1.231383	-1.432080	0.000000	4,7-didehydroquinoline						
6	1.232675	-1.436712	0.000000	6	-1.305084	-1.491124	0.000000	UBLYP/cc-pVDZ						
6	-1.304853	-1.492027	0.000000	6	2.420175	-0.753013	0.000000							

6	2.417804	-0.753101	0.000000
6	-2.426469	-0.702891	0.000000
6	2.318978	0.688746	0.000000
6	-2.462026	0.702460	0.000000
7	1.175513	1.360062	0.000000
6	-1.236194	1.374304	0.000000
1	-1.334182	-2.590857	0.000000
1	3.406956	-1.233338	0.000000
1	3.248696	1.284348	0.000000
1	-3.409608	1.260289	0.000000
1	-1.180461	2.472299	0.000000

E = -400.4288553 au
S2 = 2.00815
ZPVE = 0.105428 au
(H298 - E0) = 0.007833 au

4,7-didehydroquinoline
UBLYP/cc-pVDZ
1A' singlet state (Cs)

6	0.000000	0.704988	0.000000
6	-0.025960	-0.763848	0.000000
6	1.247729	-1.364730	0.000000
6	-1.278533	-1.457022	0.000000
6	2.427849	-0.671344	0.000000
6	-2.485857	-0.753270	0.000000
6	2.314053	0.767844	0.000000
6	-2.406992	0.651424	0.000000
7	1.161475	1.427351	0.000000
6	-1.263304	1.404729	0.000000
1	-1.272847	-2.556195	0.000000

6	-2.427898	-0.706758	0.000000
6	2.319504	0.688367	0.000000
6	-2.465203	0.699562	0.000000
7	1.176161	1.361288	0.000000
6	-1.239104	1.370352	0.000000
1	-1.331080	-2.589216	0.000000
1	3.409185	-1.233471	0.000000
1	3.248933	1.284563	0.000000
1	-3.412708	1.257189	0.000000
1	-1.187025	2.468142	0.000000

E = -400.4294172 au
S2 = 0.991144
ZPVE = 0.105283 au
(H298 - E0) = 0.007833 au

4,8-didehydroquinoline
UBLYP/cc-pVDZ
3A' triplet state (Cs)

6	0.000000	0.728170	0.000000
6	-0.059098	-0.744504	0.000000
6	-1.366074	-1.275003	0.000000
6	1.157276	-1.498329	0.000000
6	-2.500017	-0.509349	0.000000
6	2.394504	-0.863133	0.000000
6	-2.302300	0.923527	0.000000
6	2.480101	0.571793	0.000000
7	-1.117745	1.521052	0.000000
6	1.305651	1.279275	0.000000
1	1.091578	-2.594987	0.000000
1	-3.521595	-0.916294	0.000000

6	0.000000	0.707907	0.000000
6	-0.028687	-0.761741	0.000000
6	1.241677	-1.368141	0.000000
6	-1.280933	-1.454662	0.000000
6	2.425072	-0.680303	0.000000
6	-2.486520	-0.746962	0.000000
6	2.315201	0.759338	0.000000
6	-2.403419	0.656639	0.000000
7	1.166264	1.425091	0.000000
6	-1.258619	1.410591	0.000000
1	-1.276161	-2.554177	0.000000
1	3.416876	-1.154350	0.000000
1	-3.450570	-1.275283	0.000000
1	3.240201	1.362473	0.000000
1	-1.236836	2.509700	0.000000

E = -400.4298063 au
S2 = 2.011633
ZPVE = 0.105367 au
(H298 - E0) = 0.007829 au

4,8-didehydroquinoline
UBLYP/cc-pVDZ
1A' singlet state (Cs)

6	-0.055025	0.764850	0.000000
6	0.000000	-0.753147	0.000000
6	-1.265275	-1.336144	0.000000
6	1.262423	-1.423182	0.000000
6	-2.459917	-0.668990	0.000000
6	2.458269	-0.716992	0.000000

1	3.421337	-1.141969	0.000000
1	-3.448355	-1.284398	0.000000
1	3.236552	1.374881	0.000000
1	-1.240919	2.503601	0.000000

E = -400.4297091 au
S2 = 1.003119
ZPVE = 0.105290 au
(H298 - E0) = 0.007835 au

2,5-didehydroquinoline
CASSCF(12,12)/cc-pVDZ
3A' triplet state (Cs)

C	2.423167	0.552771	0.000000
C	1.269165	1.308039	0.000000
C	-0.009653	0.682983	0.000000
C	-0.103897	-0.731287	0.000000
C	1.115885	-1.444059	0.000000
C	2.357025	-0.870801	0.000000
H	3.388734	1.040506	0.000000
H	1.302446	2.387751	0.000000
C	-1.398883	-1.338659	0.000000
H	3.257720	-1.468502	0.000000
C	-2.509294	-0.532636	0.000000
C	-2.264716	0.868393	0.000000
H	-1.484674	-2.416791	0.000000
H	-3.515136	-0.924293	0.000000
N	-1.136938	1.471101	0.000000

E (CASSCF) = -398.21052530331337 au
E (CASPT2) = -399.3391628062 au

1	3.321886	-1.454798	0.000000
1	-3.191423	1.578579	0.000000
1	3.463512	1.065448	0.000000

E = -400.4236796 au
S2 = 2.009283
ZPVE = 0.105538 au
(H298 - E0) = 0.007851 au

2,5-didehydroquinoline
CASSCF(12,12)/cc-pVDZ
1A' singlet state (Cs)

C	2.425489	0.554304	0.000000
C	1.270074	1.307092	0.000000
C	-0.006537	0.678922	0.000000
C	-0.103488	-0.733889	0.000000
C	1.118912	-1.443360	0.000000
C	2.358853	-0.869305	0.000000
H	3.390584	1.042993	0.000000
H	1.300789	2.386802	0.000000
C	-1.401563	-1.337505	0.000000
H	3.259338	-1.467329	0.000000
C	-2.511464	-0.531842	0.000000
C	-2.265117	0.870115	0.000000
H	-1.489801	-2.415032	0.000000
H	-3.517184	-0.923568	0.000000
N	-1.137935	1.466117	0.000000

E (CASSCF) = -398.21036713182508 au
E (CASPT2) = -399.3409255530 au

6	-2.374093	0.769591	0.000000
6	2.440604	0.715590	0.000000
7	-1.237638	1.449575	0.000000
6	1.218325	1.337552	0.000000
1	1.257416	-2.520276	0.000000
1	-3.442219	-1.162118	0.000000
1	3.420117	-1.249594	0.000000
1	-3.304480	1.363075	0.000000
1	3.380767	1.287124	0.000000

E = -400.4363697 au
S2 = 0.590646
ZPVE = 0.104830 au
(H298 - E0) = 0.007911 au

2,6-didehydroquinoline
CASSCF(12,12)/cc-pVDZ
3A' triplet state (Cs)

C	-0.011189	0.694207	0.000000
C	-0.016242	-0.721966	0.000000
C	-1.279147	-1.396895	0.000000
C	1.231549	-1.418716	0.000000
C	-2.437182	-0.661615	0.000000
C	2.376940	-0.674087	0.000000
C	-2.276380	0.751004	0.000000
C	2.421388	0.734296	0.000000
N	-1.184694	1.414450	0.000000
C	1.218999	1.411462	0.000000
H	-1.305924	-2.478935	0.000000
H	1.253058	-2.500081	0.000000
H	-3.417141	-1.114329	0.000000

2,6-didehydroquinoline				2,7-didehydroquinoline			
CASSCF(12,12)/cc-pVDZ				CASSCF(12,12)/cc-pVDZ			
1A' singlet state (Cs)				3A' triplet state (Cs)			
C	-0.011825	0.694803	0.000000	C	-0.028416	-0.746894	0.000000
C	-0.016090	-0.722676	0.000000	C	-0.002388	0.670171	0.000000
C	-1.279067	-1.397222	0.000000	C	-1.252990	1.367083	0.000000
C	1.230942	-1.418641	0.000000	C	1.251235	1.352139	0.000000
C	-2.436980	-0.661542	0.000000	C	-2.425866	0.655045	0.000000
C	2.377557	-0.674302	0.000000	C	2.437558	0.647405	0.000000
C	-2.276935	0.750974	0.000000	C	-2.292475	-0.759823	0.000000
C	2.421186	0.734532	0.000000	C	2.358545	-0.759473	0.000000
N	-1.183518	1.414258	0.000000	N	-1.212919	-1.444329	0.000000
C	1.219179	1.411817	0.000000	C	1.195688	-1.477371	0.000000
H	-1.306295	-2.479203	0.000000	H	-1.260160	2.449465	0.000000
H	1.252483	-2.499949	0.000000	H	1.259437	2.434441	0.000000
H	-3.416762	-1.114581	0.000000	H	-3.396608	1.126994	0.000000
H	3.363684	1.263490	0.000000	H	3.392202	1.154104	0.000000
H	1.175892	2.491426	0.000000	H	1.166410	-2.556926	0.000000

E (CASSCF) = -398.21086570519623 au
E (CASPT2) = -399.3401040837 au

2,8-didehydroquinoline			
CASSCF(12,12)/cc-pVDZ			
3A' triplet state (Cs)			
C	-0.119259	-0.754240	0.000000
C	-0.002298	0.657575	0.000000
C	-1.208544	1.429398	0.000000
C	1.296520	1.249164	0.000000
C	-2.419958	0.785141	0.000000

E (CASSCF) = -398.21031814000372 au
E (CASPT2) = -399.3394000440 au

2,8-didehydroquinoline			
CASSCF(12,12)/cc-pVDZ			
1A' singlet state (Cs)			
C	-0.116634	-0.756990	0.000000
C	-0.001150	0.656563	0.000000
C	-1.208759	1.427549	0.000000
C	1.295330	1.248552	0.000000
C	-2.420931	0.786267	0.000000
C	2.434538	0.469495	0.000000

H	3.363922	1.263257	0.000000
H	1.175492	2.491134	0.000000

E (CASSCF) = -398.21002966463482 au
E (CASPT2) = -399.3389879508 au

2,7-didehydroquinoline			
CASSCF(12,12)/cc-pVDZ			
1A' singlet state (Cs)			
C	-0.027254	-0.746262	0.000000
C	-0.002037	0.670237	0.000000
C	-1.251951	1.367991	0.000000
C	1.250742	1.353906	0.000000
C	-2.424077	0.655411	0.000000
C	2.436236	0.648240	0.000000
C	-2.289207	-0.759147	0.000000
C	2.355298	-0.758193	0.000000
N	-1.213742	-1.449107	0.000000
C	1.195196	-1.478730	0.000000
H	-1.258626	2.450443	0.000000
H	1.258007	2.436335	0.000000
H	-3.395448	1.125882	0.000000
H	3.391702	1.153286	0.000000
H	1.164416	-2.558262	0.000000

E (CASSCF) = -398.21079542607015 au
E (CASPT2) = -399.3416134064 au

4,5-didehydroquinoline
CASSCF(12,12)/cc-pVDZ
3A' triplet state (Cs)

C	2.433680	0.470275	0.000000
C	-2.372056	-0.636043	0.000000
C	2.332439	-0.951251	0.000000
N	-1.338301	-1.387662	0.000000
C	1.081046	-1.500966	0.000000
H	-1.152159	2.510377	0.000000
H	1.377681	2.328146	0.000000
H	-3.361775	1.312634	0.000000
H	3.410053	0.935894	0.000000
H	3.219597	-1.569184	0.000000

E (CASSCF) = -398.20749093634709 au
E (CASPT2) = -399.3356322145 au

4,5-didehydroquinoline
CASSCF(12,12)/cc-pVDZ
1A' singlet state (Cs)

C	0.000117	0.594286	0.000000
C	-0.057646	-0.829656	0.000000
C	-1.364591	-1.371455	0.000000
C	1.184906	-1.509100	0.000000
C	-2.488773	-0.605624	0.000000
C	2.405873	-0.901473	0.000000
C	-2.292965	0.809672	0.000000
C	2.441221	0.525589	0.000000
N	-1.117202	1.380269	0.000000
C	1.270640	1.247370	0.000000
H	-3.483152	-1.028054	0.000000
H	3.319649	-1.479126	0.000000
H	-3.153377	1.468200	0.000000
H	3.395091	1.035521	0.000000

C	-2.374010	-0.636022	0.000000
C	2.334060	-0.949994	0.000000
N	-1.340497	-1.386622	0.000000
C	1.080250	-1.498752	0.000000
H	-1.151405	2.508278	0.000000
H	1.376301	2.327510	0.000000
H	-3.361716	1.315406	0.000000
H	3.410369	0.936226	0.000000
H	3.220920	-1.568207	0.000000

E (CASSCF) = -398.20861195580716 au
E (CASPT2) = -399.3379872960 au

4,6-didehydroquinoline
CASSCF(12,12)/cc-pVDZ
3A' triplet state (Cs)

C	-0.000697	0.627556	0.000000
C	-0.035334	-0.792144	0.000000
C	1.229345	-1.424343	0.000000
C	-1.291123	-1.475224	0.000000
C	2.406550	-0.740664	0.000000
C	-2.419026	-0.707048	0.000000
C	2.303214	0.684687	0.000000
C	-2.436809	0.704802	0.000000
N	1.168139	1.335369	0.000000
C	-1.225809	1.362534	0.000000
H	-1.325394	-2.555343	0.000000
H	3.371163	-1.227373	0.000000
H	3.205813	1.284323	0.000000
H	-3.370856	1.248700	0.000000
H	-1.165595	2.441442	0.000000

C	-0.000688	0.615751	0.000000
C	-0.056778	-0.804301	0.000000
C	-1.349216	-1.369975	0.000000
C	1.169602	-1.505716	0.000000
C	-2.482979	-0.614436	0.000000
C	2.397763	-0.908371	0.000000
C	-2.295168	0.802424	0.000000
C	2.438272	0.519203	0.000000
N	-1.124974	1.390076	0.000000
C	1.274881	1.256993	0.000000
H	-3.475582	-1.040916	0.000000
H	3.310165	-1.488035	0.000000
H	-3.162155	1.452512	0.000000
H	3.396394	1.021522	0.000000
H	1.293148	2.337137	0.000000

E (CASSCF) = -398.20475922473071 au
E (CASPT2) = -399.3294179713 au

4,6-didehydroquinoline
CASSCF(12,12)/cc-pVDZ
1A' singlet state (Cs)

C	0.000351	0.628827	0.000000
C	-0.032411	-0.791819	0.000000
C	1.227161	-1.422952	0.000000
C	-1.290757	-1.474571	0.000000
C	2.407279	-0.740379	0.000000
C	-2.420109	-0.708102	0.000000
C	2.304107	0.683119	0.000000
C	-2.437411	0.704811	0.000000
N	1.167715	1.335339	0.000000

H 1.272894 2.327446 0.000000

E (CASSCF) = -398.20438990822709 au

E (CASPT2) = -399.3315482887 au

4,7-didehydroquinoline

CASSCF(12,12)/cc-pVDZ

3A' triplet state (Cs)

C	-0.002513	0.680623	0.000000
C	-0.029751	-0.740260	0.000000
C	1.239075	-1.361103	0.000000
C	-1.273046	-1.442850	0.000000
C	2.412794	-0.669595	0.000000
C	-2.461825	-0.745919	0.000000
C	2.299090	0.753848	0.000000
C	-2.393586	0.664536	0.000000
N	1.158949	1.397590	0.000000
C	-1.241077	1.395488	0.000000
H	-1.264498	-2.524205	0.000000
H	3.380677	-1.149568	0.000000
H	-3.413443	-1.258278	0.000000
H	3.197078	1.360405	0.000000
H	-1.224379	2.475407	0.000000

E (CASSCF) = -398.20538545576858 au

E (CASPT2) = -399.3304633077 au

4,8-didehydroquinoline

CASSCF(12,12)/cc-pVDZ

1A' singlet state (Cs)

C	-0.004141	0.703985	0.000000
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E (CASSCF) = -398.20485362754880 au

E (CASPT2) = -399.3298946179 au

4,7-didehydroquinoline

CASSCF(12,12)/cc-pVDZ

1A' singlet state (Cs)

C	-0.002123	0.679846	0.000000
C	-0.029721	-0.740097	0.000000
C	1.240204	-1.360923	0.000000
C	-1.273412	-1.442647	0.000000
C	2.412971	-0.669908	0.000000
C	-2.461988	-0.745912	0.000000
C	2.298967	0.754056	0.000000
C	-2.393498	0.664846	0.000000
N	1.159011	1.397286	0.000000
C	-1.241652	1.395329	0.000000
H	-1.264996	-2.523897	0.000000
H	3.381012	-1.149485	0.000000
H	-3.413629	-1.258121	0.000000
H	3.196977	1.360578	0.000000
H	-1.224575	2.475169	0.000000

E (CASSCF) = -398.20465651895216 au

E (CASPT2) = -399.3306722503 au

2,4-didehydroquinoline

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 1.30 A

6	0.000000	0.652237	0.000000
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C -1.226572 1.361851 0.000000

H -1.325461 -2.554318 0.000000

H 3.371656 -1.227350 0.000000

H 3.206378 1.283104 0.000000

H -3.371166 1.249066 0.000000

H -1.167178 2.440648 0.000000

E (CASSCF) = -398.20556930876336 au

E (CASPT2) = -399.3310813013 au

4,8-didehydroquinoline

CASSCF(12,12)/cc-pVDZ

3A' triplet state (Cs)

C	0.000800	0.695502	0.000000
C	-0.054950	-0.722885	0.000000
C	-1.360594	-1.267026	0.000000
C	1.151205	-1.487044	0.000000
C	-2.485855	-0.500189	0.000000
C	2.376944	-0.859926	0.000000
C	-2.284265	0.915302	0.000000
C	2.460716	0.565822	0.000000
N	-1.108194	1.489707	0.000000
C	1.294802	1.276338	0.000000
H	1.084875	-2.566116	0.000000
H	-3.482838	-0.916664	0.000000
H	3.285869	-1.446435	0.000000
H	-3.144352	1.574408	0.000000
H	3.422093	1.060652	0.000000

E (CASSCF) = -398.20150975197890 au

E (CASPT2) = -399.3251877889 au

1	-3.183237	-1.507624	0.000000
7	1.424663	-1.231624	0.000000
6	1.317384	1.159211	0.000000
6	2.668826	1.099827	0.000000
1	3.567405	1.703092	0.000000
6	2.102390	-0.118978	0.000000

E = -400.7073005 au

E (CASPT2) = -399.7167060920 au

2,4-didehydroquinoline

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 1.80 A

6	0.000000	0.665474	0.000000
6	-0.135811	-0.766588	0.000000
6	1.295037	1.224921	0.000000
6	0.988580	-1.599621	0.000000
6	2.390749	0.392607	0.000000
6	2.233995	-1.007736	0.000000
1	1.410289	2.299244	0.000000
1	0.866691	-2.672944	0.000000
1	3.387261	0.812254	0.000000
1	3.117247	-1.633007	0.000000
7	-1.455729	-1.168416	0.000000
6	-1.216680	1.359362	0.000000
6	-2.545400	1.148982	0.000000
1	-3.442409	1.751132	0.000000
6	-2.201968	-0.147027	0.000000

E = -400.7128348 au

1	-3.159097	-1.556062	0.000000
7	1.436875	-1.207837	0.000000
6	1.281466	1.233999	0.000000
6	2.627535	1.121544	0.000000
1	3.523971	1.728019	0.000000
6	2.132586	-0.120842	0.000000

E = -400.7086786 au

E (CASPT2) = -399.7187937083 au

2,4-didehydroquinoline

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 1.90 A

6	0.000000	0.674681	0.000000
6	-0.142377	-0.757851	0.000000
6	1.303556	1.216869	0.000000
6	0.974915	-1.599896	0.000000
6	2.392947	0.376673	0.000000
6	2.226275	-1.021649	0.000000
1	1.427972	2.290012	0.000000
1	0.841490	-2.671785	0.000000
1	3.392166	0.789911	0.000000
1	3.103393	-1.655322	0.000000
7	-1.459922	-1.157536	0.000000
6	-1.192397	1.407345	0.000000
6	-2.511017	1.148697	0.000000
1	-3.410995	1.743262	0.000000
6	-2.240997	-0.177091	0.000000

E = -400.7163422 au

6	1.007397	-1.593826	0.000000
6	2.388584	0.417472	0.000000
6	2.245379	-0.984817	0.000000
1	1.388049	2.314881	0.000000
1	0.901637	-2.668828	0.000000
1	3.380871	0.846960	0.000000
1	3.136262	-1.599431	0.000000
7	-1.447936	-1.185490	0.000000
6	-1.246814	1.301796	0.000000
6	-2.584976	1.139749	0.000000
1	-3.480665	1.745861	0.000000
6	-2.165490	-0.128600	0.000000

E = -400.7101414 au

E (CASPT2) = -399.7210944757 au

2,4-didehydroquinoline

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 2.00 A

6	0.000000	0.686589	0.000000
6	-0.147300	-0.748235	0.000000
6	1.310194	1.214476	0.000000
6	0.966293	-1.594719	0.000000
6	2.395473	0.369156	0.000000
6	2.222213	-1.027310	0.000000
1	1.441552	2.286660	0.000000
1	0.824363	-2.665512	0.000000
1	3.396273	0.778610	0.000000
1	3.094497	-1.667396	0.000000
7	-1.460717	-1.152804	0.000000

E (CASPT2) = -399.7248711296 au

2,4-didehydroquinoline

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 2.10 A

6	0.000000	0.700504	0.000000
6	0.150050	-0.737375	0.000000
6	-1.314050	1.219433	0.000000
6	-0.964176	-1.583000	0.000000
6	-2.398182	0.372798	0.000000
6	-2.222763	-1.022352	0.000000
1	-1.448735	2.291147	0.000000
1	-0.818024	-2.653247	0.000000
1	-3.399167	0.781843	0.000000
1	-3.092291	-1.665959	0.000000
7	1.456687	-1.155353	0.000000
6	1.163797	1.476953	0.000000
6	2.459243	1.119773	0.000000
1	3.370630	1.691846	0.000000
6	2.324544	-0.273094	0.000000

E = -400.7213963 au

E (CASPT2) = -399.7374666061 au

2,4,5-tridehydroquinolinium cation (4)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.30 A

6	0.000000	0.706127	0.000000
6	0.038778	-0.731395	0.000000

E (CASPT2) = -399.7296768884 au

2,4-didehydroquinoline

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 2.20 A

6	0.000000	-0.716643	0.000000
6	0.150218	0.722005	0.000000
6	-1.312582	-1.238805	0.000000
6	-0.972349	1.558667	0.000000
6	-2.400369	-0.397666	0.000000
6	-2.230015	0.997726	0.000000
1	-1.443649	-2.311120	0.000000
1	-0.828415	2.629316	0.000000
1	-3.399290	-0.811760	0.000000
1	-3.100630	1.639706	0.000000
7	1.443478	1.172776	0.000000
6	1.166628	-1.488928	0.000000
6	2.444897	-1.075195	0.000000
1	3.363143	-1.635357	0.000000
6	2.370988	0.352136	0.000000

E = -400.7220082 au

E (CASPT2) = -399.7382713399 au

2,4,5-tridehydroquinolinium cation (4)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.40 A

6	0.000000	0.709050	0.000000
6	0.033722	-0.727614	0.000000

6	-1.174076	1.447522	0.000000
6	-2.482144	1.139512	0.000000
1	-3.387473	1.723273	0.000000
6	-2.281352	-0.217993	0.000000

E = -400.7195712 au

E (CASPT2) = -399.7342880301 au

2,4-didehydroquinoline

UB3LYP/cc-pVTZ

1A' singlet state (Cs)

dehydrocarbon atom separation: 2.30 A

6	0.153579	-0.717841	0.000000
6	0.000000	0.723865	0.000000
6	-1.021205	-1.501327	0.000000
6	-1.277082	1.298973	0.000000
6	-2.262672	-0.910000	0.000000
6	-2.390402	0.488878	0.000000
1	-0.923659	-2.577331	0.000000
1	-1.360916	2.376065	0.000000
1	-3.150848	-1.526870	0.000000
1	-3.375868	0.934659	0.000000
7	1.153176	1.463209	0.000000
6	1.457407	-1.231899	0.000000
6	2.595226	-0.505245	0.000000
1	3.614576	-0.849321	0.000000
6	2.265898	0.921318	0.000000

E = -400.7201582 au

E (CASPT2) = -399.7356812214 au

6	1.206601	1.369797	0.000000
6	1.229863	-1.425067	0.000000
6	2.412676	0.735418	0.000000
6	2.406247	-0.673477	0.000000
1	1.266652	-2.504714	0.000000
1	3.349140	1.275875	0.000000
1	3.355327	-1.193072	0.000000
7	-1.311627	-1.210534	0.000000
1	-1.609958	-2.174396	0.000000
6	-1.396585	0.995103	0.000000
6	-2.749067	1.054605	0.000000
1	-3.679161	1.601745	0.000000
6	-2.065281	-0.119727	0.000000

E = -400.3823319 au

E (CASPT2) = -399.3877953734 au

2,4,5-tridehydroquinolinium cation (4)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.60 A

6	0.000000	0.712952	0.000000
6	0.021044	-0.719726	0.000000
6	1.232700	1.346684	0.000000
6	1.197803	-1.444504	0.000000
6	2.421406	0.688438	0.000000
6	2.387812	-0.723675	0.000000
1	1.205352	-2.524870	0.000000
1	3.368892	1.209771	0.000000
1	3.325963	-1.262632	0.000000
7	-1.319048	-1.178953	0.000000

6	1.215283	1.363260	0.000000
6	1.220571	-1.430783	0.000000
6	2.415879	0.721453	0.000000
6	2.401085	-0.688564	0.000000
1	1.248610	-2.510729	0.000000
1	3.355863	1.255926	0.000000
1	3.346887	-1.214078	0.000000
7	-1.313147	-1.203847	0.000000
1	-1.596874	-2.173589	0.000000
6	-1.376103	1.049639	0.000000
6	-2.726467	1.061293	0.000000
1	-3.656978	1.609467	0.000000
6	-2.101549	-0.147745	0.000000

E = -400.3935545 au

E (CASPT2) = -399.4000758704 au

2,4,5-tridehydroquinolinium cation (4)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.70 A

6	0.015117	-0.717552	0.000000
6	0.000000	0.713240	0.000000
6	1.267918	-1.316095	0.000000
6	1.157613	1.471014	0.000000
6	2.437280	-0.626551	0.000000
6	2.366260	0.785326	0.000000
1	1.133217	2.551221	0.000000
1	3.398357	-1.122522	0.000000
1	3.289384	1.349569	0.000000
7	-1.344193	1.139400	0.000000

2,4,5-tridehydroquinolinium cation (4)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.50 A

6	0.000000	0.710758	0.000000
6	0.027556	-0.724135	0.000000
6	1.224240	1.354649	0.000000
6	1.209279	-1.438229	0.000000
6	2.418846	0.704493	0.000000
6	2.394572	-0.706602	0.000000
1	1.227186	-2.518424	0.000000
1	3.362675	1.232290	0.000000
1	3.336578	-1.238847	0.000000
7	-1.316181	-1.192387	0.000000
1	-1.587565	-2.167114	0.000000
6	-1.353344	1.104086	0.000000
6	-2.696974	1.070532	0.000000
1	-3.626435	1.621410	0.000000
6	-2.140703	-0.172654	0.000000

E = -400.3931236 au

E (CASPT2) = -399.4005800603 au

2,4,5-tridehydroquinolinium cation (4)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.80 A

6	0.010260	-0.726445	0.000000
6	0.000000	0.703497	0.000000
6	1.264338	-1.326432	0.000000
6	1.161819	1.458054	0.000000

1	-1.577536	-2.158499	0.000000
6	-1.330102	1.154518	0.000000
6	-2.663713	1.077390	0.000000
1	-3.591618	1.630763	0.000000
6	-2.183236	-0.199055	0.000000

E = -400.3885864 au

E (CASPT2) = -399.3974074906 au

2,4,5-tridehydroquinolinium cation (4)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.90 A

6	0.005436	-0.739803	0.000000
6	0.000000	0.691025	0.000000
6	1.260379	-1.340421	0.000000
6	1.167369	1.439960	0.000000
6	2.432659	-0.660445	0.000000
6	2.371651	0.753600	0.000000
1	1.144768	2.520497	0.000000
1	3.389901	-1.163977	0.000000
1	3.297572	1.313004	0.000000
7	-1.322600	1.151001	0.000000
1	-1.519398	2.147356	0.000000
6	-1.271558	-1.273217	0.000000
6	-2.571708	-1.059212	0.000000
1	-3.498251	-1.609597	0.000000
6	-2.320292	0.311131	0.000000

E = -400.3786545 au

E (CASPT2) = -399.3945278917 au

1	-1.606566	2.119012	0.000000
6	-1.283680	-1.224978	0.000000
6	-2.607944	-1.131240	0.000000
1	-3.523191	-1.704183	0.000000
6	-2.232872	0.185354	0.000000

E = -400.3839987 au

E (CASPT2) = -399.3947802315 au

2,4,5-tridehydroquinolinium cation (4)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.00 A

6	-0.000196	-0.755801	0.000000
6	0.000000	0.677163	0.000000
6	1.253951	-1.358254	0.000000
6	1.174845	1.417031	0.000000
6	2.429899	-0.686270	0.000000
6	2.376283	0.728279	0.000000
1	1.156386	2.497825	0.000000
1	3.383933	-1.195901	0.000000
1	3.304298	1.284073	0.000000
7	-1.309521	1.166031	0.000000
1	-1.466588	2.169958	0.000000
6	-1.271853	-1.294481	0.000000
6	-2.559492	-1.008870	0.000000
1	-3.492747	-1.545934	0.000000
6	-2.356544	0.385830	0.000000

E = -400.376645 au

E (CASPT2) = -399.3951464079 au

6	2.434691	-0.641052	0.000000
6	2.368214	0.772139	0.000000
1	1.137774	2.538405	0.000000
1	3.394197	-1.140175	0.000000
1	3.292710	1.334038	0.000000
7	-1.334038	1.142495	0.000000
1	-1.566285	2.130525	0.000000
6	-1.275421	-1.250484	0.000000
6	-2.587563	-1.099793	0.000000
1	-3.508011	-1.662435	0.000000
6	-2.278358	0.244212	0.000000

E = -400.3807811 au

E (CASPT2) = -399.3939987365 au

2,4,5-tridehydroquinolinium cation (4)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.10 A

6	-0.016150	-0.778642	0.000000
6	0.000000	0.656106	0.000000
6	1.240015	-1.384529	0.000000
6	1.185587	1.384044	0.000000
6	2.420896	-0.724841	0.000000
6	2.381210	0.690953	0.000000
1	1.172874	2.465146	0.000000
1	3.369423	-1.244833	0.000000
1	3.313262	1.239826	0.000000
7	-1.283244	1.197722	0.000000
1	-1.392429	2.208127	0.000000
6	-1.284843	-1.329875	0.000000

2,4,5-tridehydroquinolinium cation (4)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 2.20 A

6	-0.031967	-0.799215	0.000000
6	0.000000	0.638455	0.000000
6	1.220902	-1.412673	0.000000
6	1.198867	1.348514	0.000000
6	2.410194	-0.770249	0.000000
6	2.387184	0.646027	0.000000
1	1.197754	2.429905	0.000000
1	3.351758	-1.302790	0.000000
1	3.324564	1.185678	0.000000
7	-1.258073	1.235725	0.000000
1	-1.313619	2.250625	0.000000
6	-1.301172	-1.357859	0.000000
6	-2.547646	-0.832653	0.000000
1	-3.499526	-1.336522	0.000000
6	-2.378766	0.560159	0.000000

E = -400.3745819 au

E (CASPT2) = -399.3929210051 au

2,4,6-tridehydroquinolinium cation (5)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 1.40 A

6	0.000000	0.690982	0.000000
6	-0.125504	-0.734562	0.000000
6	-1.147724	1.504123	0.000000

2,4,5-tridehydroquinolinium cation (4)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 2.30 A

6	-0.048621	-0.820306	0.000000
6	0.000000	0.621914	0.000000
6	1.199410	-1.442420	0.000000
6	1.213359	1.310709	0.000000
6	2.398208	-0.819345	0.000000
6	2.393530	0.596811	0.000000
1	1.226501	2.392236	0.000000
1	3.331880	-1.365619	0.000000
1	3.336774	1.126084	0.000000
7	-1.231182	1.277320	0.000000
1	-1.229073	2.293894	0.000000
6	-1.321380	-1.380926	0.000000
6	-2.539489	-0.750926	0.000000
1	-3.505006	-1.229583	0.000000
6	-2.385484	0.658114	0.000000

E = -400.3709173 au

E (CASPT2) = -399.3873440543 au

2,4,6-tridehydroquinolinium cation (5)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 1.50 A

6	0.000000	0.692701	0.000000
6	-0.118320	-0.731985	0.000000
6	-1.158918	1.495110	0.000000

6	-2.555524	-0.917149	0.000000
1	-3.495726	-1.441777	0.000000
6	-2.368640	0.468842	0.000000

E = -400.3756237 au

E (CASPT2) = -399.3953885017 au

2,4,6-tridehydroquinolinium cation (5)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 1.30 A

6	0.000000	0.688060	0.000000
6	-0.131697	-0.737473	0.000000
6	-1.136913	1.511186	0.000000
6	-1.359462	-1.369969	0.000000
6	-2.315951	0.826326	0.000000
6	-2.488970	-0.542457	0.000000
1	-1.067943	2.590195	0.000000
1	-1.458396	-2.446294	0.000000
1	-3.478284	-0.981075	0.000000
7	1.182239	-1.310725	0.000000
1	1.412062	-2.292897	0.000000
6	1.417134	0.881303	0.000000
6	2.770417	0.848266	0.000000
1	3.735721	1.330672	0.000000
6	2.008969	-0.276164	0.000000

E = -400.3830587 au

E (CASPT2) = -399.3901711038 au

2,4,6-tridehydroquinolinium cation (5)

6	-1.349302	-1.377349	0.000000
6	-2.320322	0.811229	0.000000
6	-2.484089	-0.559846	0.000000
1	-1.086188	2.583549	0.000000
1	-1.438820	-2.454548	0.000000
1	-3.470309	-1.005367	0.000000
7	1.185068	-1.303501	0.000000
1	1.400568	-2.290404	0.000000
6	1.399690	0.937470	0.000000
6	2.747744	0.858256	0.000000
1	3.713062	1.342591	0.000000
6	2.043875	-0.305521	0.000000

E = -400.3945059 au

E (CASPT2) = -399.4014558889 au

2,4,6-tridehydroquinolinium cation (5)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.70 A

6	0.000000	0.699618	0.000000
6	-0.103530	-0.722408	0.000000
6	-1.178910	1.482593	0.000000
6	-1.314858	-1.397592	0.000000
6	-2.331501	0.764854	0.000000
6	-2.466276	-0.612903	0.000000
1	-1.140758	2.562853	0.000000
1	-1.372782	-2.477142	0.000000
1	-3.442253	-1.080339	0.000000
7	1.196727	-1.265679	0.000000
1	1.370420	-2.264636	0.000000

6	-1.337374	-1.386446	0.000000
6	-2.324584	0.793402	0.000000
6	-2.478085	-0.580034	0.000000
1	-1.105621	2.574919	0.000000
1	-1.416197	-2.464524	0.000000
1	-3.460781	-1.033254	0.000000
7	1.189631	-1.291719	0.000000
1	1.392979	-2.282660	0.000000
6	1.380050	0.993374	0.000000
6	2.718508	0.870912	0.000000
1	3.682545	1.358822	0.000000
6	2.081997	-0.332247	0.000000

E = -400.3942869 au

E (CASPT2) = -399.4021426702 au

2,4,6-tridehydroquinolinium cation (5)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.80 A

6	0.000000	0.708380	0.000000
6	-0.096739	-0.713453	0.000000
6	-1.186905	1.483158	0.000000
6	-1.306465	-1.394987	0.000000
6	-2.334306	0.759451	0.000000
6	-2.462196	-0.619814	0.000000
1	-1.154699	2.563502	0.000000
1	-1.356055	-2.475074	0.000000
1	-3.435347	-1.092989	0.000000
7	1.196894	-1.257778	0.000000
1	1.348245	-2.261172	0.000000

UB3LYP/cc-pVTZ			
2A' doublet state (Cs)			
dehydrocarbon atom separation: 1.60 A			
6	0.000000	0.694908	0.000000
6	-0.110765	-0.728401	0.000000
6	-1.169674	1.486773	0.000000
6	-1.325175	-1.394392	0.000000
6	-2.328438	0.776383	0.000000
6	-2.471765	-0.599327	0.000000
1	-1.124595	2.566876	0.000000
1	-1.393023	-2.473268	0.000000
1	-3.450849	-1.060260	0.000000
7	1.194253	-1.277854	0.000000
1	1.384878	-2.272634	0.000000
6	1.359548	1.045105	0.000000
6	2.685360	0.881510	0.000000
1	3.647536	1.372906	0.000000
6	2.123622	-0.360666	0.000000

E = -400.3899307 au

E (CASPT2) = -399.3991336923 au

2,4,6-tridehydroquinolinium cation (5)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.90 A

6	-0.091481	-0.715444	0.000000
6	0.000000	0.707612	0.000000
6	-1.373210	-1.324588	0.000000
6	-1.113080	1.540511	0.000000
6	-2.414552	-0.456951	0.000000

6	1.340710	1.088608	0.000000
6	2.652148	0.884170	0.000000
1	3.613253	1.376297	0.000000
6	2.168054	-0.396485	0.000000

E = -400.385485 au

E (CASPT2) = -399.3966358347 au

2,4,6-tridehydroquinolinium cation (5)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.00 A

6	-0.085487	-0.731818	0.000000
6	0.000000	0.693248	0.000000
6	-1.368651	-1.343470	0.000000
6	-1.121337	1.517869	0.000000
6	-2.413121	-0.481766	0.000000
6	-2.366413	0.903408	0.000000
1	-1.473414	-2.418963	0.000000
1	-1.030344	2.595594	0.000000
1	-3.270317	1.498004	0.000000
7	1.332586	1.109726	0.000000
1	1.544529	2.103210	0.000000
6	1.153136	-1.340370	0.000000
6	2.457335	-1.127462	0.000000
1	3.356211	-1.720392	0.000000
6	2.335410	0.272772	0.000000

E = -400.3782558 au

E (CASPT2) = -399.3971504177 au

6	1.325162	1.125779	0.000000
6	2.622208	0.876111	0.000000
1	3.583267	1.366104	0.000000
6	2.211963	-0.440613	0.000000

E = -400.3823533 au

E (CASPT2) = -399.3959276531 au

2,4,6-tridehydroquinolinium cation (5)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.10 A

6	-0.072807	-0.749654	0.000000
6	0.000000	0.676855	0.000000
6	-1.355631	-1.367919	0.000000
6	-1.132691	1.489451	0.000000
6	-2.407339	-0.517444	0.000000
6	-2.372597	0.868825	0.000000
1	-1.450476	-2.444312	0.000000
1	-1.049767	2.568014	0.000000
1	-3.280593	1.457029	0.000000
7	1.313949	1.139170	0.000000
1	1.483584	2.140893	0.000000
6	1.156718	-1.377097	0.000000
6	2.453054	-1.048116	0.000000
1	3.358448	-1.630767	0.000000
6	2.354820	0.347592	0.000000

E = -400.3773385 au

E (CASPT2) = -399.3971564918 au

6	-2.360729	0.927641	0.000000
1	-1.483384	-2.399680	0.000000
1	-1.018422	2.617736	0.000000
1	-3.262675	1.525356	0.000000
7	1.344950	1.093805	0.000000
1	1.595444	2.077775	0.000000
6	1.155417	-1.316223	0.000000
6	2.466396	-1.180604	0.000000
1	3.358988	-1.784458	0.000000
6	2.297139	0.202485	0.000000

E = -400.3802483 au

E (CASPT2) = -399.3964573476 au

2,4,6-tridehydroquinolinium cation (5)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.20 A

6	-0.059944	-0.770061	0.000000
6	0.000000	0.660068	0.000000
6	-1.340139	-1.395201	0.000000
6	-1.145567	1.457583	0.000000
6	-2.401083	-0.557392	0.000000
6	-2.380015	0.829132	0.000000
1	-1.424785	-2.472557	0.000000
1	-1.072618	2.537092	0.000000
1	-3.292526	1.410207	0.000000
7	1.294155	1.174949	0.000000
1	1.414488	2.183956	0.000000
6	1.166375	-1.409219	0.000000
6	2.447610	-0.970854	0.000000

2,4,6-tridehydroquinolinium cation (5)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 2.30 A

6	-0.046638	-0.791432	0.000000
6	0.000000	0.644022	0.000000
6	-1.323335	-1.424408	0.000000
6	-1.159518	1.424021	0.000000
6	-2.394213	-0.600203	0.000000
6	-2.387897	0.786316	0.000000
1	-1.396236	-2.502717	0.000000
1	-1.098378	2.504508	0.000000
1	-3.305491	1.359207	0.000000
7	1.273353	1.214320	0.000000
1	1.339463	2.228524	0.000000
6	1.179613	-1.437421	0.000000
6	2.442213	-0.897108	0.000000
1	3.373367	-1.439462	0.000000
6	2.385409	0.521164	0.000000

E = -400.3719653 au

E (CASPT2) = -399.3888051597 au

2,4,7-tridehydroquinolinium cation (6)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 1.50 A

6	0.000000	0.637535	0.000000
6	-0.127052	-0.787852	0.000000
6	-1.138968	1.459308	0.000000
6	-1.362202	-1.419408	0.000000

2,4,7-tridehydroquinolinium cation (6)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 1.30 A

6	0.000000	0.633343	0.000000
6	-0.141261	-0.793028	0.000000
6	-1.117282	1.474806	0.000000
6	-1.384917	-1.402348	0.000000
6	-2.373489	0.880773	0.000000
6	-2.418421	-0.497996	0.000000
1	-1.004453	2.549848	0.000000
1	-1.531881	-2.473733	0.000000
1	-3.274255	1.478400	0.000000
7	1.166907	-1.377044	0.000000
1	1.388864	-2.361102	0.000000
6	1.415954	0.813559	0.000000
6	2.770233	0.771146	0.000000
1	3.738843	1.246659	0.000000
6	2.001606	-0.347049	0.000000

E = -400.3848938 au

E (CASPT2) = -399.3921959947 au

2,4,7-tridehydroquinolinium cation (6)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 1.60 A

6	0.000000	0.639484	0.000000
6	-0.119019	-0.784497	0.000000
6	-1.149555	1.451202	0.000000
6	-1.349616	-1.427802	0.000000

1	3.364392	-1.536040	0.000000
6	2.371424	0.431394	0.000000

E = -400.3760204 au

E (CASPT2) = -399.3945493432 au

2,4,7-tridehydroquinolinium cation (6)
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 1.40 A

6	0.000000	0.636049	0.000000
6	-0.134691	-0.790255	0.000000
6	-1.127928	1.468043	0.000000
6	-1.374475	-1.409962	0.000000
6	-2.378390	0.865609	0.000000
6	-2.413797	-0.514496	0.000000
1	-1.022379	2.543768	0.000000
1	-1.512478	-2.482621	0.000000
1	-3.283681	1.456449	0.000000
7	1.170517	-1.370024	0.000000
1	1.378080	-2.358676	0.000000
6	1.399432	0.869588	0.000000
6	2.748063	0.781071	0.000000
1	3.716592	1.258749	0.000000
6	2.036828	-0.376898	0.000000

E = -400.3962763 au

E (CASPT2) = -399.4032118082 au

2,4,7-tridehydroquinolinium cation (6)
UB3LYP/cc-pVTZ

6	-2.383199	0.847546	0.000000
6	-2.408085	-0.533872	0.000000
1	-1.041535	2.535723	0.000000
1	-1.489883	-2.493425	0.000000
1	-3.293328	1.430988	0.000000
7	1.175948	-1.358419	0.000000
1	1.371369	-2.350973	0.000000
6	1.380713	0.925538	0.000000
6	2.719396	0.793738	0.000000
1	3.686548	1.275252	0.000000
6	2.075264	-0.403972	0.000000

E = -400.3960038 au

E (CASPT2) = -399.4038251712 au

2,4,7-tridehydroquinolinium cation (6)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.80 A

6	0.000000	0.652324	0.000000
6	-0.104095	-0.770258	0.000000
6	-1.166309	1.447889	0.000000
6	-1.330081	-1.429456	0.000000
6	-2.394043	0.812705	0.000000
6	-2.392678	-0.571905	0.000000
1	-1.089505	2.525677	0.000000
1	-1.429282	-2.506864	0.000000
1	-3.315622	1.378172	0.000000
7	1.185317	-1.325037	0.000000
1	1.329302	-2.329472	0.000000
6	1.327756	1.059211	0.000000

6	-2.387544	0.830177	0.000000
6	-2.402050	-0.552467	0.000000
1	-1.060249	2.528230	0.000000
1	-1.466613	-2.503123	0.000000
1	-3.302312	1.406400	0.000000
7	1.181427	-1.344710	0.000000
1	1.364220	-2.340949	0.000000
6	1.361049	0.977503	0.000000
6	2.686788	0.804444	0.000000
1	3.651985	1.289700	0.000000
6	2.117109	-0.432594	0.000000

E = -400.391605 au

E (CASPT2) = -399.4007716712 au

2,4,7-tridehydroquinolinium cation (6)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.90 A

6	0.000000	0.664917	0.000000
6	-0.096781	-0.759077	0.000000
6	-1.173280	1.452814	0.000000
6	-1.322511	-1.422148	0.000000
6	-2.397141	0.812387	0.000000
6	-2.389580	-0.572645	0.000000
1	-1.101466	2.530860	0.000000
1	-1.414749	-2.500365	0.000000
1	-3.320996	1.374197	0.000000
7	1.184184	-1.322916	0.000000
1	1.300763	-2.331524	0.000000
6	1.315972	1.093230	0.000000

2A' doublet state (Cs)
dehydrocarbon atom separation: 1.70 A

6	0.000000	0.643895	0.000000
6	-0.111281	-0.778894	0.000000
6	-1.158844	1.446684	0.000000
6	-1.338496	-1.431919	0.000000
6	-2.391185	0.817586	0.000000
6	-2.396680	-0.566127	0.000000
1	-1.076692	2.524183	0.000000
1	-1.445715	-2.508381	0.000000
1	-3.309862	1.387645	0.000000
7	1.184986	-1.332475	0.000000
1	1.351499	-2.332613	0.000000
6	1.342676	1.022448	0.000000
6	2.654033	0.807558	0.000000
1	3.617714	1.294456	0.000000
6	2.161136	-0.467559	0.000000

E = -400.387118 au

E (CASPT2) = -399.3982237485 au

2,4,7-tridehydroquinolinium cation (6)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.00 A

6	0.000000	0.680399	0.000000
6	-0.087709	-0.745930	0.000000
6	-1.181048	1.458858	0.000000
6	-1.312932	-1.413445	0.000000
6	-2.400625	0.812347	0.000000
6	-2.384949	-0.572773	0.000000

6	2.624284	0.799291	0.000000
1	3.588052	1.283788	0.000000
6	2.205139	-0.512476	0.000000

E = -400.3839331 au

E (CASPT2) = -399.3974551525 au

2,4,7-tridehydroquinolinium cation (6)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.10 A

6	0.000000	0.696923	0.000000
6	-0.072672	-0.731101	0.000000
6	-1.192935	1.459598	0.000000
6	-1.294430	-1.409167	0.000000
6	-2.405820	0.802743	0.000000
6	-2.375021	-0.582389	0.000000
1	-1.137639	2.538745	0.000000
1	-1.366409	-2.489296	0.000000
1	-3.338003	1.350711	0.000000
7	1.186043	-1.330869	0.000000
1	1.248911	-2.344777	0.000000
6	1.290688	1.192967	0.000000
6	2.546013	0.726409	0.000000
1	3.507113	1.211448	0.000000
6	2.301465	-0.647774	0.000000

E = -400.3788422 au

E (CASPT2) = -399.3984336941 au

2,4,8-tridehydroquinolinium cation (7)

6	2.598338	0.781790	0.000000
1	3.562907	1.262211	0.000000
6	2.245691	-0.563762	0.000000

E = -400.3817466 au

E (CASPT2) = -399.3979232239 au

2,4,7-tridehydroquinolinium cation (6)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.20 A

6	0.000000	-0.715977	0.000000
6	-0.057312	0.715593	0.000000
6	-1.203921	-1.462663	0.000000
6	-1.277338	1.401015	0.000000
6	-2.411058	-0.796826	0.000000
6	-2.366216	0.587805	0.000000
1	-1.158483	-2.542416	0.000000
1	-1.338233	2.482043	0.000000
1	-3.348012	-1.336601	0.000000
7	1.188099	1.342315	0.000000
1	1.219600	2.357822	0.000000
6	1.279170	-1.247958	0.000000
6	2.518644	-0.698679	0.000000
1	3.480203	-1.183606	0.000000
6	2.322737	0.688783	0.000000

E = -400.3776197 au

E (CASPT2) = -399.3956861751 au

2,4,8-tridehydroquinolinium cation (7)

1	-1.115168	2.537281	0.000000
1	-1.397366	-2.492510	0.000000
1	-3.327370	1.369458	0.000000
7	1.183190	-1.325353	0.000000
1	1.270936	-2.337338	0.000000
6	1.305144	1.132564	0.000000
6	2.574149	0.756322	0.000000
1	3.538471	1.235344	0.000000
6	2.279330	-0.614136	0.000000

E = -400.3796936 au

E (CASPT2) = -399.3985831013 au

2,4,7-tridehydroquinolinium cation (6)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.30 A

6	-0.045034	-0.735198	0.000000
6	0.000000	0.701533	0.000000
6	-1.301149	-1.390862	0.000000
6	-1.174845	1.465166	0.000000
6	-2.460038	-0.644862	0.000000
6	-2.317908	0.732531	0.000000
1	-1.331134	-2.471302	0.000000
1	-1.160579	2.547996	0.000000
1	-3.431893	-1.118931	0.000000
7	1.269864	1.282275	0.000000
1	1.328434	2.296772	0.000000
6	1.188116	-1.373574	0.000000
6	2.447763	-0.823813	0.000000
1	3.380961	-1.362622	0.000000

UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 1.30 A

6	0.000000	0.618849	0.000000
6	0.043887	-0.817298	0.000000
6	1.179336	1.366638	0.000000
6	1.259674	-1.427044	0.000000
6	2.387003	0.688797	0.000000
6	2.434091	-0.720539	0.000000
1	1.147392	2.446348	0.000000
1	3.315900	1.241037	0.000000
1	3.391148	-1.226591	0.000000
7	-1.293356	-1.322489	0.000000
1	-1.568720	-2.293284	0.000000
6	-1.405982	0.881931	0.000000
6	-2.760122	0.922473	0.000000
1	-3.698265	1.455763	0.000000
6	-2.060213	-0.241449	0.000000

E = -400.3822383 au

E (CASPT2) = -399.3874013035 au

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.60 A

6	0.000000	0.627747	0.000000
6	0.020415	-0.804811	0.000000
6	1.210837	1.340208	0.000000
6	1.221824	-1.450778	0.000000
6	2.397026	0.633919	0.000000

UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 1.40 A

6	0.000000	0.622401	0.000000
6	0.037025	-0.813268	0.000000
6	1.189689	1.359021	0.000000
6	1.248576	-1.434198	0.000000
6	2.390624	0.672322	0.000000
6	2.427672	-0.738651	0.000000
1	1.166030	2.438877	0.000000
1	3.323980	1.217086	0.000000
1	3.381005	-1.251764	0.000000
7	-1.296806	-1.314542	0.000000
1	-1.558347	-2.290651	0.000000
6	-1.385897	0.937957	0.000000
6	-2.737199	0.932336	0.000000
1	-3.674946	1.468117	0.000000
6	-2.097170	-0.267899	0.000000

E = -400.3936444 au

E (CASPT2) = -399.3997830824 au

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.70 A

6	0.000000	0.633083	0.000000
6	0.012755	-0.797943	0.000000
6	1.219335	1.335849	0.000000
6	1.210971	-1.452920	0.000000
6	2.399341	0.621912	0.000000

6 2.383956 0.591106 0.000000

E = -400.3736843 au

E (CASPT2) = -399.3898102121 au

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.50 A

6	0.000000	0.624809	0.000000
6	0.028895	-0.809516	0.000000
6	1.200502	1.349241	0.000000
6	1.235317	-1.443174	0.000000
6	2.394037	0.652642	0.000000
6	2.419737	-0.759948	0.000000
1	1.186116	2.429172	0.000000
1	3.332217	1.189133	0.000000
1	3.368759	-1.281056	0.000000
7	-1.302058	-1.301681	0.000000
1	-1.552144	-2.282273	0.000000
6	-1.363395	0.993946	0.000000
6	-2.707380	0.944985	0.000000
1	-3.643256	1.484988	0.000000
6	-2.137261	-0.291018	0.000000

E = -400.3934114 au

E (CASPT2) = -399.4003896678 au

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

6	2.411516	-0.780178	0.000000
1	1.205625	2.420114	0.000000
1	3.339795	1.162373	0.000000
1	3.356118	-1.309304	0.000000
7	-1.307168	-1.286852	0.000000
1	-1.545166	-2.271797	0.000000
6	-1.340227	1.045725	0.000000
6	-2.673725	0.955091	0.000000
1	-3.607237	1.499056	0.000000
6	-2.180827	-0.315668	0.000000

E = -400.3890973 au

E (CASPT2) = -399.3973428549 au

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.90 A

6	0.000000	0.656444	0.000000
6	-0.000728	-0.776055	0.000000
6	1.232815	1.342447	0.000000
6	1.196577	-1.437527	0.000000
6	2.404156	0.618621	0.000000
6	2.397408	-0.798536	0.000000
1	1.245129	2.421915	0.000000
1	3.354877	1.132830	0.000000
1	3.332063	-1.344945	0.000000
7	-1.306936	-1.266397	0.000000
1	-1.477124	-2.267913	0.000000
6	-1.289914	1.157072	0.000000
6	-2.587567	0.922639	0.000000

6	2.404828	-0.793590	0.000000
1	1.221370	2.415641	0.000000
1	3.345745	1.143925	0.000000
1	3.345750	-1.329282	0.000000
7	-1.309606	-1.274569	0.000000
1	-1.530956	-2.264513	0.000000
6	-1.319484	1.088782	0.000000
6	-2.640695	0.955952	0.000000
1	-3.573110	1.500613	0.000000
6	-2.227312	-0.348524	0.000000

E = -400.3847744 au

E (CASPT2) = -399.3948546398 au

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.00 A

6	0.000000	0.674732	0.000000
6	-0.010758	-0.761896	0.000000
6	1.240854	1.348920	0.000000
6	1.186720	-1.424792	0.000000
6	2.407216	0.619464	0.000000
6	2.392170	-0.797933	0.000000
1	1.259394	2.428210	0.000000
1	3.360610	1.128732	0.000000
1	3.322213	-1.352012	0.000000
7	-1.304801	-1.270079	0.000000
1	-1.445684	-2.276654	0.000000
6	-1.276820	1.196763	0.000000
6	-2.565113	0.890025	0.000000

dehydrocarbon atom separation: 1.80 A

6	0.000000	0.642549	0.000000
6	0.005995	-0.788255	0.000000
6	1.226497	1.336763	0.000000
6	1.202848	-1.448397	0.000000
6	2.401629	0.617113	0.000000
6	2.400298	-0.799424	0.000000
1	1.234287	2.416402	0.000000
1	3.350553	1.134592	0.000000
1	3.338014	-1.340670	0.000000
7	-1.309315	-1.267315	0.000000
1	-1.507931	-2.262920	0.000000
6	-1.302730	1.124875	0.000000
6	-2.611766	0.944964	0.000000
1	-3.544293	1.487455	0.000000
6	-2.273674	-0.390799	0.000000

E = -400.3818707 au

E (CASPT2) = -399.3942397218 au

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.10 A

6	0.000000	0.693895	0.000000
6	-0.024287	-0.745821	0.000000
6	1.250133	1.353565	0.000000
6	1.172534	-1.412807	0.000000
6	2.410540	0.617147	0.000000
6	2.383636	-0.800681	0.000000
1	1.276375	2.432711	0.000000

1	-3.521275	1.460900	0.000000
6	-2.316933	-0.441438	0.000000

E = -400.3801614 au

E (CASPT2) = -399.3949772644 au

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.20 A

6	0.000000	0.714264	0.000000
6	-0.037334	-0.728966	0.000000
6	1.258006	1.359796	0.000000
6	1.159821	-1.398096	0.000000
6	2.413905	0.617627	0.000000
6	2.376421	-0.799972	0.000000
1	1.291583	2.438793	0.000000
1	3.374319	1.113576	0.000000
1	3.295106	-1.372390	0.000000
7	-1.304199	-1.292591	0.000000
1	-1.380045	-2.306473	0.000000
6	-1.252401	1.298643	0.000000
6	-2.518029	0.817538	0.000000
1	-3.450142	1.357287	0.000000
6	-2.400628	-0.577943	0.000000

E = -400.3787005 au

E (CASPT2) = -399.3939370465 au

2,4,5-tridehydroquinoline

UB3LYP/cc-pVTZ

1	-3.497449	1.429064	0.000000
6	-2.351848	-0.489747	0.000000

E = -400.3791747 au

E (CASPT2) = -399.3960594406 au

2,4,8-tridehydroquinolinium cation (7)

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.30 A

6	-0.051166	-0.732986	0.000000
6	0.000000	0.714847	0.000000
6	1.166775	-1.451710	0.000000
6	1.241654	1.298965	0.000000
6	2.368241	-0.786615	0.000000
6	2.419794	0.630186	0.000000
1	1.131597	-2.530776	0.000000
1	3.295030	-1.343003	0.000000
1	3.371391	1.145961	0.000000
7	-1.209596	1.398066	0.000000
1	-1.177855	2.414392	0.000000
6	-1.333703	-1.257175	0.000000
6	-2.545035	-0.609735	0.000000
1	-3.516426	-1.076461	0.000000
6	-2.372654	0.794794	0.000000

E = -400.3752432 au

E (CASPT2) = -399.3886773150 au

2,4,5-tridehydroquinoline

UB3LYP/cc-pVTZ

1	3.367825	1.119099	0.000000
1	3.307932	-1.364161	0.000000
7	-1.304562	-1.278543	0.000000
1	-1.415704	-2.289038	0.000000
6	-1.262882	1.248848	0.000000
6	-2.541253	0.852894	0.000000
1	-3.471387	1.395423	0.000000
6	-2.377273	-0.531077	0.000000

E = -400.3793202 au

E (CASPT2) = -399.3961744951 au

2,4,5-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.30 A

6	0.000000	0.705877	0.000000
6	0.059063	-0.755765	0.000000
6	-1.237474	1.308443	0.000000
6	-1.135256	-1.482429	0.000000
6	-2.412873	0.621032	0.000000
6	-2.336234	-0.793833	0.000000
1	-1.111840	-2.562559	0.000000
1	-3.375337	1.113598	0.000000
1	-3.263548	-1.353915	0.000000
7	1.375116	-1.237501	0.000000
6	1.381641	1.040221	0.000000
6	2.733167	1.077521	0.000000
1	3.640173	1.662612	0.000000
6	2.028757	-0.087272	0.000000

2A' doublet state (Cs)
dehydrocarbon atom separation: 1.40 A

6	0.000000	0.707907	0.000000
6	0.067064	-0.751701	0.000000
6	-1.250234	1.293754	0.000000
6	-1.119079	-1.494102	0.000000
6	-2.416490	0.594515	0.000000
6	-2.326674	-0.820742	0.000000
1	-1.081086	-2.573703	0.000000
1	-3.384025	1.077353	0.000000
1	-3.248114	-1.390259	0.000000
7	1.380331	-1.225057	0.000000
6	1.353764	1.111666	0.000000
6	2.706932	1.088799	0.000000
1	3.615936	1.674072	0.000000
6	2.057212	-0.098772	0.000000

E = -400.0126627 au

E (CASPT2) = -399.0243452958 au

2,4,5-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.70 A

6	0.000000	0.709588	0.000000
6	-0.096410	-0.738983	0.000000
6	1.287002	1.233759	0.000000
6	1.054891	-1.536274	0.000000
6	2.425101	0.494311	0.000000
6	2.288205	-0.917477	0.000000
1	0.964521	-2.612476	0.000000

2A' doublet state (Cs)
dehydrocarbon atom separation: 1.50 A

6	0.000000	0.707993	0.000000
6	-0.076626	-0.748068	0.000000
6	1.263445	1.274161	0.000000
6	1.098554	-1.509138	0.000000
6	2.419862	0.561220	0.000000
6	2.314431	-0.853560	0.000000
1	1.043349	-2.587886	0.000000
1	3.393008	1.032900	0.000000
1	3.228610	-1.434470	0.000000
7	-1.389478	-1.205836	0.000000
6	-1.321805	1.187061	0.000000
6	-2.671901	1.106763	0.000000
1	-3.580262	1.694882	0.000000
6	-2.085688	-0.103862	0.000000

E = -400.0173614 au

E (CASPT2) = -399.0299345405 au

2,4,5-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.80 A

6	0.000000	0.714465	0.000000
6	-0.104260	-0.732273	0.000000
6	1.295879	1.219832	0.000000
6	1.037797	-1.542479	0.000000
6	2.427297	0.470714	0.000000
6	2.278290	-0.939177	0.000000
1	0.933208	-2.617337	0.000000

E = -399.9968264 au
E (CASPT2) = -399.0073797792 au

2,4,5-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.60 A

6	0.000000	0.707871	0.000000
6	-0.086875	-0.744110	0.000000
6	1.276063	1.252778	0.000000
6	1.075985	-1.524433	0.000000
6	2.422727	0.525781	0.000000
6	2.300847	-0.887741	0.000000
1	1.002586	-2.602000	0.000000
1	3.401420	0.986032	0.000000
1	3.206988	-1.480916	0.000000
7	-1.400513	-1.183493	0.000000
6	-1.287493	1.261334	0.000000
6	-2.631031	1.127061	0.000000
1	-3.537768	1.717823	0.000000
6	-2.115164	-0.107958	0.000000

E = -400.0183941 au

E (CASPT2) = -399.0318184199 au

2,4,5-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.90 A

6	0.000000	0.722856	0.000000
6	-0.110293	-0.724095	0.000000

1	3.408554	0.944428	0.000000
1	3.186533	-1.522217	0.000000
7	-1.410502	-1.162708	0.000000
6	-1.254358	1.328580	0.000000
6	-2.588941	1.143696	0.000000
1	-3.495060	1.734033	0.000000
6	-2.147329	-0.118003	0.000000

E = -400.0195698 au
E (CASPT2) = -399.0339797173 au

2,4,5-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 2.00 A

6	-0.116418	-0.724883	0.000000
6	0.000000	0.724101	0.000000
6	1.100523	-1.399900	0.000000
6	1.248214	1.357519	0.000000
6	2.330652	-0.827762	0.000000
6	2.391477	0.586676	0.000000
1	1.295277	2.436368	0.000000
1	3.240037	-1.413419	0.000000
1	3.361212	1.067868	0.000000
7	-1.224642	1.341689	0.000000
6	-1.403336	-1.268593	0.000000
6	-2.635106	-0.735655	0.000000
1	-3.629062	-1.150895	0.000000
6	-2.198501	0.566540	0.000000

E = -400.0286973 au

1	3.414322	0.913032	0.000000
1	3.169767	-1.553770	0.000000
7	-1.417535	-1.146581	0.000000
6	-1.225492	1.385903	0.000000
6	-2.549531	1.152390	0.000000
1	-3.457108	1.738095	0.000000
6	-2.182887	-0.138366	0.000000

E = -400.0220595 au
E (CASPT2) = -399.0377107480 au

2,4,5-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 2.10 A

6	0.121539	-0.736072	0.000000
6	0.000000	0.714481	0.000000
6	-1.093033	-1.412845	0.000000
6	-1.253355	1.337938	0.000000
6	-2.326887	-0.848941	0.000000
6	-2.394727	0.564360	0.000000
1	-1.305074	2.416595	0.000000
1	-3.232542	-1.440355	0.000000
1	-3.365841	1.042585	0.000000
7	1.212419	1.350504	0.000000
6	1.404849	-1.286945	0.000000
6	2.611832	-0.704235	0.000000
1	3.611550	-1.102126	0.000000
6	2.230611	0.643888	0.000000

E = -400.0308444 au

6	1.302921	1.211587	0.000000
6	1.025445	-1.542758	0.000000
6	2.429655	0.455776	0.000000
6	2.271728	-0.952246	0.000000
1	0.909745	-2.616440	0.000000
1	3.419046	0.892841	0.000000
1	3.157550	-1.574760	0.000000
7	-1.421137	-1.136169	0.000000
6	-1.202284	1.433919	0.000000
6	-2.514909	1.151867	0.000000
1	-3.425899	1.729426	0.000000
6	-2.221011	-0.169888	0.000000

E = -400.025463 au
E (CASPT2) = -399.0425634822 au

2,4,5-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 2.20 A

6	-0.132837	-0.761496	0.000000
6	0.000000	0.692737	0.000000
6	1.084404	-1.437440	0.000000
6	1.262555	1.302221	0.000000
6	2.321367	-0.884083	0.000000
6	2.400932	0.528182	0.000000
1	1.315752	2.380890	0.000000
1	3.220780	-1.485043	0.000000
1	3.374317	1.001274	0.000000
7	-1.183234	1.374792	0.000000
6	-1.425179	-1.295137	0.000000

E (CASPT2) = -399.0472946340 au

2,4,5-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.30 A

6	-0.141552	-0.780236	0.000000
6	0.000000	0.677853	0.000000
6	1.072553	-1.459368	0.000000
6	1.271053	1.271221	0.000000
6	2.314681	-0.918448	0.000000
6	2.405494	0.492194	0.000000
1	1.331085	2.349597	0.000000
1	3.208211	-1.528140	0.000000
1	3.381549	0.959512	0.000000
7	-1.160517	1.397184	0.000000
6	-1.440111	-1.306563	0.000000
6	-2.581582	-0.585986	0.000000
1	-3.596692	-0.942518	0.000000
6	-2.267292	0.839543	0.000000

E = -400.0295935 au

E (CASPT2) = -399.0492179529 au

2,4,6-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.50 A

6	0.000000	0.682327	0.000000
6	-0.012109	-0.763812	0.000000
6	-1.213406	1.410766	0.000000

E (CASPT2) = -399.0506902602 au

2,4,6-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.30 A

6	0.000000	0.679804	0.000000
6	-0.032873	-0.768778	0.000000
6	-1.179959	1.446919	0.000000
6	-1.264649	-1.434402	0.000000
6	-2.326662	0.714391	0.000000
6	-2.425803	-0.669821	0.000000
1	-1.160718	2.528386	0.000000
1	-1.304170	-2.514719	0.000000
1	-3.393729	-1.154874	0.000000
7	1.249439	-1.345714	0.000000
6	1.403539	0.926611	0.000000
6	2.754368	0.873492	0.000000
1	3.697149	1.399365	0.000000
6	1.974605	-0.241244	0.000000

E = -399.9951107 au

E (CASPT2) = -399.0077893209 au

2,4,6-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.60 A

6	0.000000	0.682504	0.000000
6	-0.000572	-0.761184	0.000000
6	-1.229884	1.388721	0.000000

6	-2.597548	-0.640052	0.000000
1	-3.605802	-1.014753	0.000000
6	-2.250762	0.744082	0.000000

E = -400.0311861 au

E (CASPT2) = -399.0516298358 au

2,4,6-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.40 A

6	0.000000	0.682040	0.000000
6	-0.023148	-0.766027	0.000000
6	-1.196401	1.431166	0.000000
6	-1.246897	-1.448893	0.000000
6	-2.332186	0.685470	0.000000
6	-2.416556	-0.700912	0.000000
1	-1.189866	2.512647	0.000000
1	-1.270279	-2.529589	0.000000
1	-3.378689	-1.197171	0.000000
7	1.256934	-1.332366	0.000000
6	1.379143	1.001176	0.000000
6	2.728061	0.889119	0.000000
1	3.672380	1.415777	0.000000
6	2.002636	-0.252321	0.000000

E = -400.0114919 au

E (CASPT2) = -399.0243723757 au

2,4,6-tridehydroquinoline

UB3LYP/cc-pVTZ

6	-1.225309	-1.466665	0.000000
6	-2.337736	0.650488	0.000000
6	-2.405104	-0.737519	0.000000
1	-1.221052	2.492083	0.000000
1	-1.230119	-2.547518	0.000000
1	-3.360305	-1.246796	0.000000
7	1.268608	-1.312973	0.000000
6	1.351153	1.079372	0.000000
6	2.693738	0.911304	0.000000
1	3.637177	1.441435	0.000000
6	2.031114	-0.257660	0.000000

E = -400.0167124 au
E (CASPT2) = -399.0303300092 au

2,4,6-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 1.80 A

6	0.000000	0.689885	0.000000
6	0.019556	-0.751054	0.000000
6	-1.256734	1.354629	0.000000
6	-1.160739	-1.507549	0.000000
6	-2.351208	0.554849	0.000000
6	-2.370632	-0.833962	0.000000
1	-1.305506	2.434343	0.000000
1	-1.112368	-2.587155	0.000000
1	-3.303841	-1.381856	0.000000
7	1.304239	-1.253660	0.000000
6	1.264980	1.285554	0.000000
6	2.573356	0.970262	0.000000

6	-1.201731	-1.484720	0.000000
6	-2.342881	0.613535	0.000000
6	-2.392414	-0.775384	0.000000
1	-1.252425	2.469649	0.000000
1	-1.187250	-2.565402	0.000000
1	-3.339944	-1.298596	0.000000
7	1.282385	-1.290793	0.000000
6	1.320750	1.156207	0.000000
6	2.653853	0.936059	0.000000
1	3.595365	1.469600	0.000000
6	2.060806	-0.262355	0.000000

E = -400.0181889 au
E (CASPT2) = -399.0324607076 au

2,4,6-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 1.90 A

6	0.000000	0.698401	0.000000
6	0.027171	-0.743369	0.000000
6	-1.266742	1.345699	0.000000
6	-1.146266	-1.509963	0.000000
6	-2.354763	0.537414	0.000000
6	-2.363583	-0.850661	0.000000
1	-1.325595	2.424778	0.000000
1	-1.085208	-2.588917	0.000000
1	-3.290963	-1.408113	0.000000
7	1.309992	-1.242413	0.000000
6	1.243507	1.336037	0.000000
6	2.538059	0.974415	0.000000

2A' doublet state (Cs)
dehydrocarbon atom separation: 1.70 A

6	0.000000	0.684637	0.000000
6	0.010211	-0.757085	0.000000
6	-1.244477	1.369178	0.000000
6	-1.179433	-1.499121	0.000000
6	-2.347317	0.580465	0.000000
6	-2.380415	-0.808658	0.000000
1	-1.281100	2.449533	0.000000
1	-1.146938	-2.579343	0.000000
1	-3.320399	-1.345093	0.000000
7	1.294947	-1.270120	0.000000
6	1.291102	1.225820	0.000000
6	2.612575	0.957126	0.000000
1	3.553016	1.490934	0.000000
6	2.092887	-0.273227	0.000000

E = -400.0196962 au
E (CASPT2) = -399.0347532391 au

2,4,6-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 2.00 A

6	0.000000	0.709781	0.000000
6	0.033347	-0.734515	0.000000
6	-1.274933	1.341783	0.000000
6	-1.135675	-1.507193	0.000000
6	-2.358203	0.527244	0.000000
6	-2.359132	-0.859786	0.000000
1	-1.342010	2.420284	0.000000

1	3.514565	1.500083	0.000000
6	2.127669	-0.294246	0.000000

E = -400.0223928 au
E (CASPT2) = -399.0384955869 au

2,4,6-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 2.10 A

6	0.000000	-0.723667	0.000000
6	0.037884	0.723426	0.000000
6	-1.280194	-1.346330	0.000000
6	-1.131129	1.496039	0.000000
6	-2.361351	-0.529339	0.000000
6	-2.358617	0.856586	0.000000
1	-1.351692	-2.424396	0.000000
1	-1.055745	2.574086	0.000000
1	-3.277790	1.426966	0.000000
7	1.309981	1.237479	0.000000
6	1.216799	-1.408945	0.000000
6	2.481381	-0.955049	0.000000
1	3.433097	-1.457245	0.000000
6	2.242270	0.423652	0.000000

E = -400.0309723 au
E (CASPT2) = -399.0510496639 au

2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

1	3.481686	1.496864	0.000000
6	2.164306	-0.325928	0.000000

E = -400.0258854 au
E (CASPT2) = -399.0432633678 au

2,4,6-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 2.20 A

6	0.043357	-0.738790	0.000000
6	0.000000	0.709236	0.000000
6	-1.199486	-1.433786	0.000000
6	-1.217704	1.405277	0.000000
6	-2.327553	-0.684253	0.000000
6	-2.406980	0.699271	0.000000
1	-1.207074	-2.514314	0.000000
1	-1.203300	2.486006	0.000000
1	-3.357151	1.216056	0.000000
7	1.223784	1.321964	0.000000
6	1.297500	-1.351578	0.000000
6	2.510781	-0.774899	0.000000
1	3.494443	-1.210161	0.000000
6	2.251184	0.630967	0.000000

E = -400.03162 au
E (CASPT2) = -399.0518242018 au

2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

1	-1.064939	-2.585558	0.000000
1	-3.281580	-1.425109	0.000000
7	1.312616	-1.236194	0.000000
6	1.226710	1.379151	0.000000
6	2.507220	0.970663	0.000000
1	3.454380	1.483761	0.000000
6	2.201640	-0.367134	0.000000

E = -400.0291013 au
E (CASPT2) = -399.0478457249 au

2,4,6-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 2.30 A

6	0.049242	-0.756112	0.000000
6	0.000000	0.695189	0.000000
6	-1.190562	-1.455144	0.000000
6	-1.225804	1.377800	0.000000
6	-2.324227	-0.714007	0.000000
6	-2.412713	0.667822	0.000000
1	-1.192086	-2.535791	0.000000
1	-1.217663	2.458648	0.000000
1	-3.364920	1.180644	0.000000
7	1.206227	1.343250	0.000000
6	1.306993	-1.367473	0.000000
6	2.496483	-0.726945	0.000000
1	3.486842	-1.147465	0.000000
6	2.274627	0.719075	0.000000

E = -400.0297713 au

dehydrocarbon atom separation: 1.30 A

6	0.000000	0.627041	0.000000
6	-0.036547	-0.824760	0.000000
6	-1.161952	1.405948	0.000000
6	-1.284815	-1.473559	0.000000
6	-2.386508	0.753973	0.000000
6	-2.358119	-0.633600	0.000000
1	-1.107714	2.486686	0.000000
1	-1.360381	-2.552114	0.000000
1	-3.316126	1.305373	0.000000
7	1.238134	-1.408882	0.000000
6	1.403949	0.863705	0.000000
6	2.755666	0.803800	0.000000
1	3.701566	1.323720	0.000000
6	1.970946	-0.306130	0.000000

E = -399.9979584 au

E (CASPT2) = -399.0104124544 au

**2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)**

dehydrocarbon atom separation: 1.60 A

6	0.000000	0.628806	0.000000
6	-0.001292	-0.816914	0.000000
6	-1.211725	1.347895	0.000000
6	-1.219311	-1.525125	0.000000
6	-2.405549	0.650129	0.000000
6	-2.326678	-0.737104	0.000000
1	-1.200151	2.429352	0.000000
1	-1.240533	-2.605922	0.000000

dehydrocarbon atom separation: 1.40 A

6	0.000000	0.628884	0.000000
6	-0.026191	-0.821986	0.000000
6	-1.177965	1.390530	0.000000
6	-1.266681	-1.488070	0.000000
6	-2.392822	0.724928	0.000000
6	-2.349655	-0.663283	0.000000
1	-1.136311	2.471646	0.000000
1	-1.326527	-2.567547	0.000000
1	-3.329026	1.265260	0.000000
7	1.246958	-1.395974	0.000000
6	1.380947	0.937819	0.000000
6	2.730217	0.819461	0.000000
1	3.677392	1.340681	0.000000
6	1.999777	-0.317988	0.000000

E = -400.0140271 au

E (CASPT2) = -399.0266844338 au

**2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)**

dehydrocarbon atom separation: 1.70 A

6	0.000000	0.630749	0.000000
6	0.010938	-0.812635	0.000000
6	-1.227040	1.327713	0.000000
6	-1.195248	-1.540615	0.000000
6	-2.411073	0.614518	0.000000
6	-2.314886	-0.771259	0.000000
1	-1.230543	2.409023	0.000000
1	-1.197398	-2.621564	0.000000

E (CASPT2) = -399.0492601746 au

**2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)**

dehydrocarbon atom separation: 1.50 A

6	0.000000	0.628865	0.000000
6	-0.014153	-0.819690	0.000000
6	-1.194891	1.370218	0.000000
6	-1.244247	-1.506261	0.000000
6	-2.399330	0.688968	0.000000
6	-2.338887	-0.699137	0.000000
1	-1.167726	2.451601	0.000000
1	-1.285436	-2.586547	0.000000
1	-3.342705	1.216841	0.000000
7	1.260256	-1.376641	0.000000
6	1.354158	1.016098	0.000000
6	2.696690	0.842207	0.000000
1	3.642717	1.367476	0.000000
6	2.029219	-0.323414	0.000000

E = -400.0189495 au

E (CASPT2) = -399.0323853746 au

**2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)**

dehydrocarbon atom separation: 1.80 A

6	0.000000	0.635903	0.000000
6	0.021495	-0.806433	0.000000
6	-1.240008	1.312638	0.000000

1	-3.356132	1.165045	0.000000
7	1.275907	-1.354055	0.000000
6	1.324598	1.093613	0.000000
6	2.657421	0.868160	0.000000
1	3.601147	1.397599	0.000000
6	2.059921	-0.327408	0.000000

E = -400.0201655 au
E (CASPT2) = -399.0343091010 au

2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 1.90 A

6	0.000000	0.644356	0.000000
6	0.030203	-0.798602	0.000000
6	-1.250726	1.303241	0.000000
6	-1.158732	-1.553396	0.000000
6	-2.420218	0.567132	0.000000
6	-2.298028	-0.815034	0.000000
1	-1.278481	2.383868	0.000000
1	-1.131037	-2.633950	0.000000
1	-3.386013	1.053189	0.000000
7	1.308812	-1.303766	0.000000
6	1.247578	1.276494	0.000000
6	2.542185	0.911334	0.000000
1	3.486625	1.432102	0.000000
6	2.165609	-0.387002	0.000000

E = -400.0273074 au
E (CASPT2) = -399.0446742019 au

1	-3.368063	1.117537	0.000000
7	1.290476	-1.332612	0.000000
6	1.295296	1.164379	0.000000
6	2.616462	0.890995	0.000000
1	3.558620	1.421611	0.000000
6	2.092895	-0.336899	0.000000

E = -400.0214602 au
E (CASPT2) = -399.0364427408 au

2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

dehydrocarbon atom separation: 2.00 A

6	0.000000	0.655689	0.000000
6	0.037287	-0.789629	0.000000
6	-1.259508	1.299020	0.000000
6	-1.146825	-1.551246	0.000000
6	-2.424310	0.555466	0.000000
6	-2.293477	-0.824832	0.000000
1	-1.296218	2.379270	0.000000
1	-1.108823	-2.631494	0.000000
1	-3.392671	1.036453	0.000000
7	1.312568	-1.297302	0.000000
6	1.230575	1.320247	0.000000
6	2.511357	0.908581	0.000000
1	3.459012	1.420535	0.000000
6	2.203356	-0.427237	0.000000

E = -400.0303504 au
E (CASPT2) = -399.0491073602 au

6	-1.174803	-1.550100	0.000000
6	-2.415877	0.586572	0.000000
6	-2.305154	-0.797451	0.000000
1	-1.256728	2.393642	0.000000
1	-1.160446	-2.630925	0.000000
1	-3.377937	1.079911	0.000000
7	1.301569	-1.315511	0.000000
6	1.269224	1.225135	0.000000
6	2.577423	0.905771	0.000000
1	3.519882	1.433187	0.000000
6	2.128407	-0.356575	0.000000

E = -400.0239801 au
E (CASPT2) = -399.0400464642 au

2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 2.10 A

6	0.000000	0.669970	0.000000
6	0.041764	-0.777901	0.000000
6	-1.264149	1.304773	0.000000
6	-1.142707	-1.539362	0.000000
6	-2.427193	0.558892	0.000000
6	-2.293313	-0.820344	0.000000
1	-1.304918	2.384860	0.000000
1	-1.098794	-2.619490	0.000000
1	-3.396169	1.038697	0.000000
7	1.309091	-1.300053	0.000000
6	1.222035	1.349218	0.000000
6	2.485975	0.891010	0.000000

2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 2.20 A

6	0.000000	0.686483	0.000000
6	0.044467	-0.762241	0.000000
6	-1.263534	1.321872	0.000000
6	-1.145967	-1.516385	0.000000
6	-2.428363	0.579397	0.000000
6	-2.297211	-0.799622	0.000000
1	-1.302571	2.402195	0.000000
1	-1.101491	-2.596634	0.000000
1	-3.395773	1.062401	0.000000
7	1.297297	-1.314506	0.000000
6	1.222910	1.365090	0.000000
6	2.466516	0.852807	0.000000
1	3.423919	1.342959	0.000000
6	2.283654	-0.562297	0.000000

E = -400.0326253 au
E (CASPT2) = -399.0527703976 au

2,4,8-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 1.40 A

6	0.000000	0.608369	0.000000
6	0.075906	-0.848864	0.000000
6	-1.231083	1.280720	0.000000
6	-1.140159	-1.507208	0.000000

2,4,7-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 2.30 A

6	0.000000	0.704005	0.000000
6	0.047996	-0.748344	0.000000
6	-1.264487	1.335768	0.000000
6	-1.146163	-1.496649	0.000000
6	-2.430534	0.594592	0.000000
6	-2.299658	-0.783303	0.000000
1	-1.304121	2.416224	0.000000
1	-1.101209	-2.576956	0.000000
1	-3.397129	1.079260	0.000000
7	1.288717	-1.328559	0.000000
6	1.222608	1.388664	0.000000
6	2.449109	0.820222	0.000000
1	3.411860	1.300397	0.000000
6	2.316059	-0.634790	0.000000

E = -400.0306144 au
E (CASPT2) = -399.0499985682 au

2,4,8-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 1.50 A

6	0.000000	0.610265	0.000000
6	0.089070	-0.844173	0.000000
6	-1.247631	1.258789	0.000000
6	-1.115440	-1.525413	0.000000

1	3.438581	1.391240	0.000000
6	2.243864	-0.485411	0.000000

E = -400.0320835 au
E (CASPT2) = -399.0521701417 au

2,4,8-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)
dehydrocarbon atom separation: 1.30 A

6	0.000000	0.604635	0.000000
6	0.064464	-0.853891	0.000000
6	-1.215074	1.297721	0.000000
6	-1.160293	-1.492506	0.000000
6	-2.389815	0.573830	0.000000
6	-2.358393	-0.843156	0.000000
1	-1.229743	2.378824	0.000000
1	-3.345431	1.079734	0.000000
1	-3.291171	-1.394186	0.000000
7	1.375920	-1.350761	0.000000
6	1.387097	0.929493	0.000000
6	2.739824	0.959368	0.000000
1	3.649170	1.541074	0.000000
6	2.029813	-0.200514	0.000000

E = -399.9939189 au
E (CASPT2) = -399.0059935123 au

2,4,8-tridehydroquinoline
UB3LYP/cc-pVTZ
2A' doublet state (Cs)

6	-2.394038	0.541552	0.000000
6	-2.346055	-0.876215	0.000000
1	-1.260819	2.361337	0.000000
1	-3.356423	1.034684	0.000000
1	-3.271773	-1.438885	0.000000
7	1.384505	-1.335105	0.000000
6	1.358679	1.004400	0.000000
6	2.712928	0.976211	0.000000
1	3.623036	1.559963	0.000000
6	2.059562	-0.207526	0.000000

E = -400.010003 au

E (CASPT2) = -399.0222587191 au

2,4,8-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.70 A

6	0.000000	0.615778	0.000000
6	-0.115152	-0.832640	0.000000
6	1.277266	1.215074	0.000000
6	1.064048	-1.557409	0.000000
6	2.403286	0.425399	0.000000
6	2.297967	-0.989775	0.000000
1	1.357256	2.292510	0.000000
1	3.386196	0.876703	0.000000
1	3.196924	-1.593772	0.000000
7	-1.424749	-1.263346	0.000000
6	-1.257466	1.229808	0.000000
6	-2.593766	1.046118	0.000000
1	-3.497707	1.639712	0.000000

6	-2.397823	0.502353	0.000000
6	-2.330602	-0.915323	0.000000
1	-1.294283	2.338613	0.000000
1	-3.367526	0.981121	0.000000
1	-3.247807	-1.491607	0.000000
7	1.397353	-1.312459	0.000000
6	1.326030	1.083243	0.000000
6	2.677305	0.999933	0.000000
1	3.585468	1.588455	0.000000
6	2.089537	-0.207902	0.000000

E = -400.0150092 au

E (CASPT2) = -399.0279779846 au

2,4,8-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.80 A

6	0.000000	0.622450	0.000000
6	-0.125053	-0.824787	0.000000
6	1.288395	1.200764	0.000000
6	1.044273	-1.564476	0.000000
6	2.405420	0.398730	0.000000
6	2.285746	-1.014626	0.000000
1	1.381552	2.276929	0.000000
1	3.392881	0.840096	0.000000
1	3.176935	-1.629825	0.000000
7	-1.433672	-1.245373	0.000000
6	-1.228638	1.288099	0.000000
6	-2.554584	1.057127	0.000000
1	-3.459561	1.646764	0.000000

dehydrocarbon atom separation: 1.60 A

6	0.000000	0.612096	0.000000
6	-0.102756	-0.839017	0.000000
6	1.263493	1.235378	0.000000
6	1.088720	-1.543572	0.000000
6	2.400889	0.461347	0.000000
6	2.313646	-0.955377	0.000000
1	1.327580	2.314095	0.000000
1	3.377725	0.925536	0.000000
1	3.221550	-1.546030	0.000000
7	-1.411942	-1.286816	0.000000
6	-1.291018	1.160512	0.000000
6	-2.635992	1.025528	0.000000
1	-3.541364	1.618370	0.000000
6	-2.120631	-0.207604	0.000000

E = -400.0163873 au

E (CASPT2) = -399.0299612460 au

2,4,8-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 1.90 A

6	0.000000	0.632351	0.000000
6	-0.132337	-0.815747	0.000000
6	1.297050	1.193169	0.000000
6	1.030279	-1.564299	0.000000
6	2.407694	0.382332	0.000000
6	2.277804	-1.029179	0.000000
1	1.400341	2.268219	0.000000
1	3.398169	0.816995	0.000000

6 -2.154422 -0.214308 0.000000

E = -400.0179131 au

E (CASPT2) = -399.0321692031 au

2,4,8-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.00 A

6	0.000000	0.645059	0.000000
6	-0.137238	-0.806073	0.000000
6	1.303281	1.192429	0.000000
6	1.022340	-1.556607	0.000000
6	2.410372	0.376585	0.000000
6	2.274528	-1.033179	0.000000
1	1.413330	2.266648	0.000000
1	3.402331	0.807935	0.000000
1	3.154585	-1.663719	0.000000
7	-1.438405	-1.229775	0.000000
6	-1.190226	1.373094	0.000000
6	-2.491954	1.046536	0.000000
1	-3.405064	1.618013	0.000000
6	-2.273828	-0.307920	0.000000

E = -400.028057 au

E (CASPT2) = -399.0453515256 au

2,4,8-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.30 A

6 -2.191578 -0.232672 0.000000

E = -400.020731 au

E (CASPT2) = -399.0358814481 au

2,4,8-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.10 A

6	0.000000	0.660951	0.000000
6	-0.139150	-0.794272	0.000000
6	1.304906	1.204502	0.000000
6	1.024388	-1.536553	0.000000
6	2.412893	0.390289	0.000000
6	2.278278	-1.018663	0.000000
1	1.415188	2.278624	0.000000
1	3.403885	0.823891	0.000000
1	3.156736	-1.651137	0.000000
7	-1.430285	-1.238138	0.000000
6	-1.185485	1.392897	0.000000
6	-2.471328	1.015191	0.000000
1	-3.390428	1.574880	0.000000
6	-2.320068	-0.374225	0.000000

E = -400.0308973 au

E (CASPT2) = -399.0486968605 au

1 3.162674 -1.653209 0.000000

7 -1.438252 -1.234082 0.000000

6 -1.205993 1.335797 0.000000

6 -2.520510 1.057228 0.000000

1 -3.428765 1.639036 0.000000

6 -2.231429 -0.263729 0.000000

E = -400.0244422 au

E (CASPT2) = -399.0406712973 au

2,4,8-tridehydroquinoline

UB3LYP/cc-pVTZ

2A' doublet state (Cs)

dehydrocarbon atom separation: 2.20 A

6	0.000000	0.678031	0.000000
6	-0.141152	-0.781285	0.000000
6	1.304924	1.220874	0.000000
6	1.029320	-1.511878	0.000000
6	2.415642	0.410860	0.000000
6	2.283901	-0.997680	0.000000
1	1.412620	2.295337	0.000000
1	3.405075	0.847978	0.000000
1	3.161633	-1.630904	0.000000
7	-1.419645	-1.253032	0.000000
6	-1.185232	1.410578	0.000000
6	-2.455388	0.974509	0.000000
1	-3.380601	1.523395	0.000000
6	-2.362218	-0.448105	0.000000

E = -400.0322614 au

E (CASPT2) = -399.0495256682 au

6	0.000000	0.695874	0.000000
6	-0.143548	-0.767631	0.000000
6	1.305387	1.236023	0.000000
6	1.032486	-1.488654	0.000000
6	2.418414	0.428822	0.000000
6	2.288542	-0.978624	0.000000
1	1.412064	2.310660	0.000000
1	3.406667	0.868716	0.000000
1	3.165022	-1.613314	0.000000
7	-1.410872	-1.270314	0.000000
6	-1.185202	1.433923	0.000000
6	-2.441624	0.936273	0.000000
1	-3.372596	1.475946	0.000000
6	-2.396965	-0.520976	0.000000

E = -400.0307826 au

E (CASPT2) = -399.0471446348 au