

Supplementary Information to: Electronic Properties of Hexagonal Graphene Quantum Rings from TAO-DFT

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Cartesian coordinates for the lowest singlet states of n -HGQRs ($n = 3-15$), calculated by spin-unrestricted TAO-LDA (S2 to S47).

Cartesian coordinates for the lowest triplet states of n -HGQRs ($n = 3-15$), calculated by spin-unrestricted TAO-LDA (S48 to S93).

FIG. S1. Singlet-quintet gap of n -HGQR, calculated by spin-unrestricted TAO-LDA (S94).

TABLE S1. Singlet-triplet gap of n -HGQR, calculated by spin-unrestricted KS-LDA and TAO-LDA (S94).

TABLE S2. Vertical ionization potential, vertical electron affinity, fundamental gap, and symmetrized von Neumann entropy of ground-state n -HGQR, calculated by spin-unrestricted TAO-LDA (S95).

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Cartesian coordinates (in Å) for the lowest singlet states of n -HGQRs ($n = 3$ –15), calculated by spin-unrestricted TAO-LDA.

3-HGQR (singlet)

C	-6.14848528	-0.68184816	0.00000000
C	-6.14848532	0.68184808	0.00000000
C	-4.90417045	-2.83169560	0.00000000
C	-4.93177990	-1.43278832	0.00000000
C	-4.93177995	1.43278833	0.00000000
C	-4.90417056	2.83169561	0.00000000
C	-3.66496130	-4.98470372	0.00000000
C	-3.70680641	-3.55545297	0.00000000
C	-3.69499632	-0.72289751	0.00000000
C	-3.69499631	0.72289750	0.00000000
C	-3.70680663	3.55545296	0.00000000
C	-3.66496144	4.98470369	0.00000000
C	-2.48404937	-5.66666552	0.00000000
C	-2.47364017	-2.83939036	0.00000000
C	-2.51277813	-1.45128974	0.00000000
C	-2.51277820	1.45128979	0.00000000
C	-2.47364041	2.83939039	0.00000000
C	-2.48404945	5.66666556	0.00000000
C	-1.22533924	-4.98850315	0.00000000
C	-1.22170225	-3.56235090	0.00000000
C	-1.22170246	3.56235097	0.00000000
C	-1.22533922	4.98850324	0.00000000
C	-0.00000001	-5.66384240	0.00000000
C	0.00000000	-2.90237945	0.00000000
C	-0.00000002	2.90237935	0.00000000
C	-0.00000001	5.66384238	0.00000000
C	1.22533924	-4.98850315	0.00000000
C	1.22170226	-3.56235090	0.00000000
C	1.22170244	3.56235096	0.00000000
C	1.22533920	4.98850323	0.00000000
C	2.48404937	-5.66666553	0.00000000
C	2.47364018	-2.83939036	0.00000000
C	2.51277815	-1.45128975	0.00000000
C	2.51277820	1.45128976	0.00000000
C	2.47364040	2.83939036	0.00000000
C	2.48404943	5.66666554	0.00000000
C	3.66496131	-4.98470374	0.00000000
C	3.70680641	-3.55545298	0.00000000
C	3.69499634	-0.72289752	0.00000000
C	3.69499632	0.72289749	0.00000000
C	3.70680661	3.55545295	0.00000000
C	3.66496143	4.98470367	0.00000000
C	4.90417046	-2.83169562	0.00000000
C	4.93177992	-1.43278834	0.00000000
C	4.93177995	1.43278833	0.00000000
C	4.90417056	2.83169560	0.00000000
C	6.14848530	-0.68184815	0.00000000
C	6.14848532	0.68184808	0.00000000
H	-7.09736725	-1.23595024	0.00000000
H	-7.09736731	1.23595014	0.00000000
H	-5.85717467	-3.38178623	0.00000000
H	-5.85717483	3.38178615	0.00000000
H	-4.61926075	-5.52943853	0.00000000
H	-4.61926081	5.52943865	0.00000000
H	-2.47862582	-6.76546748	0.00000000
H	-2.47862599	6.76546754	0.00000000
H	-1.56467070	-0.90452921	0.00000000
H	-1.56467068	0.90452933	0.00000000
H	0.00000000	-6.76420128	0.00000000
H	-0.00000001	-1.80792276	0.00000000
H	-0.00000003	1.80792263	0.00000000
H	0.00000001	6.76420125	0.00000000
H	1.56467074	-0.90452920	0.00000000
H	1.56467070	0.90452929	0.00000000
H	2.47862582	-6.76546749	0.00000000
H	2.47862598	6.76546753	0.00000000
H	4.61926076	-5.52943854	0.00000000
H	4.61926079	5.52943863	0.00000000
H	5.85717468	-3.38178625	0.00000000
H	5.85717482	3.38178615	0.00000000
H	7.09736727	-1.23595023	0.00000000
H	7.09736731	1.23595014	0.00000000

4-HGQR (singlet)

C	-8.59735933	-0.67995805	0.00000000
C	-8.59735926	0.67995902	0.00000000
C	-7.38450940	-2.82689430	0.00000000
C	-7.38113439	-1.43602754	0.00000000
C	-7.38113435	1.43602829	0.00000000

C	-7.38450931	2.82689481	0.00000000
C	-6.14031201	-4.98223851	0.00000000
C	-6.19349387	-3.57611843	0.00000000
C	-6.13197078	-0.72570470	0.00000000
C	-6.13197079	0.72570545	0.00000000
C	-6.19349388	3.57611875	0.00000000
C	-6.14031195	4.98223879	0.00000000
C	-4.88749518	-7.10593705	0.00000000
C	-4.93404767	-5.67456817	0.00000000
C	-4.95125308	-2.85883836	0.00000000
C	-4.96068454	-1.45787206	0.00000000
C	-4.96068454	1.45787264	0.00000000
C	-4.95125316	2.85883879	0.00000000
C	-4.93404774	5.67456833	0.00000000
C	-4.88749534	7.10593697	0.00000000
C	-3.70990012	-7.78601699	0.00000000
C	-3.69433375	-4.94778840	0.00000000
C	-3.74261318	-3.56722204	0.00000000
C	-3.74261341	3.56722245	0.00000000
C	-3.69433409	4.94778857	0.00000000
C	-3.70990060	7.78601678	0.00000000
C	-2.44704249	-7.11077272	0.00000000
C	-2.43756522	-5.67363797	0.00000000
C	-2.43756581	5.67363801	0.00000000
C	-2.44704321	7.11077259	0.00000000
C	-1.24431808	-7.80924122	0.00000000
C	-1.21785796	-5.02537563	0.00000000
C	-1.21785881	5.02537568	0.00000000
C	-1.24431904	7.80924113	0.00000000
C	0.00000048	-7.15237183	0.00000000
C	0.00000047	-5.71775330	0.00000000
C	-0.00000047	5.71775332	0.00000000
C	-0.00000049	7.15237185	0.00000000
C	1.24431904	-7.80924110	0.00000000
C	1.21785881	-5.02537565	0.00000000
C	1.21785797	5.02537566	0.00000000
C	1.24431807	7.80924125	0.00000000
C	2.44704322	-7.11077257	0.00000000
C	2.43756580	-5.67363799	0.00000000
C	2.43756523	5.67363798	0.00000000
C	2.44704249	7.11077274	0.00000000
C	3.70990061	-7.78601677	0.00000000
C	3.69433409	-4.94778857	0.00000000
C	3.74261340	-3.56722245	0.00000000
C	3.74261319	3.56722204	0.00000000
C	3.69433375	4.94778840	0.00000000
C	3.70990012	7.78601699	0.00000000
C	4.88749536	-7.10593698	0.00000000
C	4.93404774	-5.67456834	0.00000000
C	4.95125316	-2.85883880	0.00000000
C	4.96068454	-1.45787265	0.00000000
C	4.96068453	1.45787205	0.00000000
C	4.95125309	2.85883835	0.00000000
C	4.93404767	5.67456816	0.00000000
C	4.88749517	7.10593703	0.00000000
C	6.14031196	-4.98223880	0.00000000
C	6.19349387	-3.57611876	0.00000000
C	6.13197079	-0.72570545	0.00000000
C	6.13197077	0.72570470	0.00000000
C	6.19349388	3.57611841	0.00000000
C	6.14031200	4.98223850	0.00000000
C	7.38450930	-2.82689482	0.00000000
C	7.38113435	-1.43602830	0.00000000
C	7.38113440	1.43602752	0.00000000
C	7.38450942	2.82689428	0.00000000
C	8.59735926	-0.67995903	0.00000000
C	8.59735934	0.67995804	0.00000000
H	-9.54558737	-1.23517423	0.00000000
H	-9.54558727	1.23517513	0.00000000
H	-8.34857090	-3.35688420	0.00000000
H	-8.34857072	3.35688480	0.00000000
H	-7.08119878	-5.55241172	0.00000000
H	-7.08119868	5.55241199	0.00000000
H	-5.84248661	-7.64943087	0.00000000
H	-5.84248675	7.64943073	0.00000000
H	-3.98588399	-0.95178880	0.00000000
H	-3.98588404	0.95178931	0.00000000
H	-3.70317434	-8.88480291	0.00000000
H	-3.70317484	8.88480267	0.00000000
H	-2.81692842	-2.97598936	0.00000000
H	-2.81692863	2.97598982	0.00000000
H	-1.26752800	-8.90913030	0.00000000
H	-1.16898452	-3.92814743	0.00000000

H	-1.16898528	3.92814749	0.00000000
H	-1.26752898	8.90913017	0.00000000
H	1.26752898	-8.90913015	0.00000000
H	1.16898529	-3.92814746	0.00000000
H	1.16898452	3.92814745	0.00000000
H	1.26752801	8.90913033	0.00000000
H	2.81692863	-2.97598981	0.00000000
H	2.81692842	2.97598936	0.00000000
H	3.70317483	-8.88480265	0.00000000
H	3.70317437	8.88480292	0.00000000
H	3.98588404	-0.95178933	0.00000000
H	3.98588398	0.95178879	0.00000000
H	5.84248676	-7.64943074	0.00000000
H	5.84248660	7.64943084	0.00000000
H	7.08119870	-5.55241198	0.00000000
H	7.08119876	5.55241171	0.00000000
H	8.34857071	-3.35688481	0.00000000
H	8.34857092	3.35688418	0.00000000
H	9.54558726	-1.23517515	0.00000000
H	9.54558738	1.23517422	0.00000000

5-HGQR (singlet)

C	-11.04713949	-0.67967855	0.00000000
C	-11.04713939	0.67967914	0.00000000
C	-9.84124389	-2.82215311	0.00000000
C	-9.83142003	-1.43571198	0.00000000
C	-9.83141982	1.43571235	0.00000000
C	-9.84124339	2.82215355	0.00000000
C	-8.63192208	-4.98378347	0.00000000
C	-8.65364324	-3.58391149	0.00000000
C	-8.57624459	-0.72663603	0.00000000
C	-8.57624448	0.72663617	0.00000000
C	-8.65364261	3.58391179	0.00000000
C	-8.63192124	4.98378370	0.00000000
C	-7.36422820	-7.11139688	0.00000000
C	-7.43022049	-5.70202062	0.00000000
C	-7.40102221	-2.86794294	0.00000000
C	-7.41007625	-1.46159190	0.00000000
C	-7.41007592	1.46159195	0.00000000
C	-7.40102166	2.86794311	0.00000000
C	-7.43021969	5.70202062	0.00000000
C	-7.36422737	7.11139670	0.00000000
C	-6.11166758	-9.22662573	0.00000000
C	-6.15848711	-7.79573435	0.00000000
C	-6.18405390	-4.97479348	0.00000000
C	-6.20453355	-3.58167311	0.00000000
C	-6.20453288	3.58167327	0.00000000
C	-6.18405321	4.97479356	0.00000000
C	-6.15848640	7.79573394	0.00000000
C	-6.11166694	9.22662519	0.00000000
C	-4.93453074	-9.90633113	0.00000000
C	-4.91693311	-7.06292515	0.00000000
C	-4.97043162	-5.68538830	0.00000000
C	-4.97043108	5.68538818	0.00000000
C	-4.91693257	7.06292474	0.00000000
C	-4.93453023	9.90633054	0.00000000
C	-3.67204209	-9.23136886	0.00000000
C	-3.65848973	-7.78962833	0.00000000
C	-3.65848930	7.78962783	0.00000000
C	-3.67204170	9.23136828	0.00000000
C	-2.47642571	-9.93324522	0.00000000
C	-2.43884385	-7.14729686	0.00000000
C	-2.43884356	7.14729644	0.00000000
C	-2.47642551	9.93324465	0.00000000
C	-1.22293236	-9.28571495	0.00000000
C	-1.21650750	-7.84275201	0.00000000
C	-1.21650729	7.84275156	0.00000000
C	-1.22293221	9.28571447	0.00000000
C	-0.00000003	-9.96710930	0.00000000
C	-0.00000006	-7.16365156	0.00000000
C	0.00000013	7.16365121	0.00000000
C	0.00000007	9.96710890	0.00000000
C	1.22293227	-9.28571491	0.00000000
C	1.21650739	-7.84275198	0.00000000
C	1.21650750	7.84275163	0.00000000
C	1.22293236	9.28571453	0.00000000
C	2.47642564	-9.93324515	0.00000000
C	2.43884372	-7.14729679	0.00000000
C	2.43884379	7.14729656	0.00000000
C	2.47642564	9.93324477	0.00000000
C	3.67204199	-9.23136876	0.00000000
C	3.65848961	-7.78962822	0.00000000
C	3.65848949	7.78962800	0.00000000
C	3.67204185	9.23136844	0.00000000

C	4.93453065	-9.90633101	0.00000000
C	4.91693297	-7.06292502	0.00000000
C	4.97043148	-5.68538816	0.00000000
C	4.97043122	5.68538838	0.00000000
C	4.91693275	7.06292493	0.00000000
C	4.93453038	9.90633072	0.00000000
C	6.11166748	-9.22662559	0.00000000
C	6.15848698	-7.79573421	0.00000000
C	6.18405376	-4.97479334	0.00000000
C	6.20453341	-3.58167296	0.00000000
C	6.20453295	3.58167345	0.00000000
C	6.18405333	4.97479374	0.00000000
C	6.15848658	7.79573413	0.00000000
C	6.11166709	9.22662537	0.00000000
C	7.36422807	-7.11139674	0.00000000
C	7.43022034	-5.70202048	0.00000000
C	7.40102209	-2.86794280	0.00000000
C	7.41007615	-1.46159176	0.00000000
C	7.41007590	1.46159211	0.00000000
C	7.40102170	2.86794327	0.00000000
C	7.43021982	5.70202078	0.00000000
C	7.36422754	7.11139687	0.00000000
C	8.63192194	-4.98378336	0.00000000
C	8.65364310	-3.58391137	0.00000000
C	8.57624451	-0.72663591	0.00000000
C	8.57624444	0.72663629	0.00000000
C	8.65364267	3.58391192	0.00000000
C	8.63192136	4.98378383	0.00000000
C	9.84124377	-2.82215301	0.00000000
C	9.83141993	-1.43571188	0.00000000
C	9.83141980	1.43571243	0.00000000
C	9.84124342	2.82215363	0.00000000
C	11.04713942	-0.67967849	0.00000000
C	11.04713936	0.67967920	0.00000000
H	-11.99493458	-1.23568456	0.00000000
H	-11.99493439	1.23568529	0.00000000
H	-10.80795392	-3.34744521	0.00000000
H	-10.80795331	3.34744580	0.00000000
H	-9.58436768	-5.53419846	0.00000000
H	-9.58436676	5.53419874	0.00000000
H	-8.30233310	-7.68626555	0.00000000
H	-8.30233223	7.68626539	0.00000000
H	-7.06711137	-9.76936679	0.00000000
H	-7.06711071	9.76936621	0.00000000
H	-6.43357620	-0.95839386	0.00000000
H	-6.43357596	0.95839377	0.00000000
H	-5.25188857	-3.03118569	0.00000000
H	-5.25188798	3.03118576	0.00000000
H	-4.92680005	-11.00513202	0.00000000
H	-4.92679953	11.00513139	0.00000000
H	-4.04650284	-5.09110099	0.00000000
H	-4.04650238	5.09110085	0.00000000
H	-2.50505656	-11.03307755	0.00000000
H	-2.38637661	-6.05004925	0.00000000
H	-2.38637633	6.05004890	0.00000000
H	-2.50505638	11.03307694	0.00000000
H	-0.00000001	-11.06713884	0.00000000
H	-0.00000008	-6.06343228	0.00000000
H	0.00000016	6.06343202	0.00000000
H	0.00000004	11.06713839	0.00000000
H	2.50505653	-11.03307748	0.00000000
H	2.38637644	-6.05004917	0.00000000
H	2.38637661	6.05004902	0.00000000
H	2.50505647	11.03307705	0.00000000
H	4.04650269	-5.09110086	0.00000000
H	4.04650251	5.09110107	0.00000000
H	4.92679998	-11.00513190	0.00000000
H	4.92679966	11.00513156	0.00000000
H	5.25188844	-3.03118554	0.00000000
H	5.25188803	3.03118598	0.00000000
H	6.43357611	-0.95839371	0.00000000
H	6.43357592	0.95839397	0.00000000
H	7.06711128	-9.76936663	0.00000000
H	7.06711086	9.76936641	0.00000000
H	8.30233298	-7.68626540	0.00000000
H	8.30233240	7.68626554	0.00000000
H	9.58436753	-5.53419835	0.00000000
H	9.58436690	5.53419884	0.00000000
H	10.80795379	-3.34744512	0.00000000
H	10.80795336	3.34744585	0.00000000
H	11.99493450	-1.23568454	0.00000000
H	11.99493437	1.23568533	0.00000000

6-HGQR (singlet)

C	-13.49724507	-0.67987993	0.00000000
C	-13.49724493	0.67988116	0.00000000
C	-12.29497003	-2.81979264	0.00000000
C	-12.28226189	-1.43467990	0.00000000
C	-12.28226158	1.43468085	0.00000000
C	-12.29496947	2.81979354	0.00000000
C	-11.09568159	-4.98131804	0.00000000
C	-11.10916821	-3.58538969	0.00000000
C	-11.02394811	-0.72648150	0.00000000
C	-11.02394795	0.72648219	0.00000000
C	-11.10916751	3.58539028	0.00000000
C	-11.09568070	4.98131855	0.00000000
C	-9.86147147	-7.11738630	0.00000000
C	-9.89720732	-5.71341967	0.00000000
C	-9.85185774	-2.87235649	0.00000000
C	-9.85960502	-1.46419943	0.00000000
C	-9.85960470	1.46419983	0.00000000
C	-9.85185717	2.87235684	0.00000000
C	-9.89720633	5.71341985	0.00000000
C	-9.86147034	7.11738638	0.00000000
C	-8.58841856	-9.23584067	0.00000000
C	-8.65888863	-7.82615086	0.00000000
C	-8.64137593	-4.98782581	0.00000000
C	-8.66051270	-3.58933337	0.00000000
C	-8.66051200	3.58933341	0.00000000
C	-8.64137503	4.98782577	0.00000000
C	-8.65888742	7.82615061	0.00000000
C	-8.58841728	9.23584031	0.00000000
C	-7.33603880	-11.34638678	0.00000000
C	-7.38227047	-9.91676653	0.00000000
C	-7.41310758	-7.09307960	0.00000000
C	-7.43935811	-5.70278063	0.00000000
C	-7.43935712	5.70278028	0.00000000
C	-7.41310646	7.09307917	0.00000000
C	-7.38226918	9.91676588	0.00000000
C	-7.33603742	11.34638608	0.00000000
C	-6.15849582	-12.02614535	0.00000000
C	-6.14001892	-9.18056339	0.00000000
C	-6.19710608	-7.80321729	0.00000000
C	-6.19710489	7.80321659	0.00000000
C	-6.14001773	9.18056258	0.00000000
C	-6.15849459	12.02614448	0.00000000
C	-4.89755442	-11.35101505	0.00000000
C	-4.88174463	-9.90697445	0.00000000
C	-4.88174350	9.90697352	0.00000000
C	-4.89755330	11.35101411	0.00000000
C	-3.70454377	-12.05469268	0.00000000
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7-HGQR (singlet)

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8-HGQR (singlet)			
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10-HGQR (singlet)

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11-HGQR (singlet)

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12-HGQR (singlet)

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13-HGQR (singlet)

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14-HGQR (singlet)

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15-HGQR (singlet)

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C	20.96315885	-24.80689986	0.00000000
C	20.97584801	-21.95927965	0.00000000
C	21.02322787	-20.55901703	0.00000000
C	21.02319644	20.55902432	0.00000000
C	20.97581871	21.95928326	0.00000000
C	20.96313346	24.80689432	0.00000000
C	20.90793641	26.20635677	0.00000000
C	22.17461218	-24.10121239	0.00000000
C	22.22409934	-22.70478852	0.00000000
C	22.22751486	-19.85509954	0.00000000
C	22.27072178	-18.45552189	0.00000000
C	22.27068749	18.45553542	0.00000000
C	22.22748165	19.85511053	0.00000000
C	22.22406903	22.70479132	0.00000000
C	22.17458419	24.10121066	0.00000000
C	23.43338559	-21.99336931	0.00000000
C	23.47885316	-20.59708758	0.00000000
C	23.47305535	-17.74664325	0.00000000
C	23.51126051	-16.34815388	0.00000000
C	23.51122613	16.34817132	0.00000000
C	23.47302052	17.74665947	0.00000000
C	23.47881883	20.59709853	0.00000000
C	23.43335257	21.99337614	0.00000000
C	24.68502922	-19.88187752	0.00000000
C	24.72688126	-18.48459273	0.00000000
C	24.71174566	-15.63410431	0.00000000
C	24.74461362	-14.23661356	0.00000000
C	24.74458152	14.23663337	0.00000000
C	24.71171180	15.63412365	0.00000000
C	24.72684535	18.48460982	0.00000000
C	24.68499314	19.88189201	0.00000000
C	25.92985015	-17.76629249	0.00000000
C	25.96793958	-16.36779056	0.00000000
C	25.94319729	-13.51741389	0.00000000
C	25.97052600	-12.12086331	0.00000000
C	25.97049750	12.12088538	0.00000000
C	25.94316622	13.51743546	0.00000000
C	25.96790454	16.36781136	0.00000000
C	25.92981374	17.76631220	0.00000000
C	27.16782500	-15.64645068	0.00000000
C	27.20189986	-14.24677586	0.00000000
C	27.16724261	-11.39646375	0.00000000
C	27.18881431	-10.00090810	0.00000000
C	27.18878986	10.00093326	0.00000000
C	27.16721514	11.39648802	0.00000000
C	27.20186717	14.24679908	0.00000000
C	27.16779024	15.64647349	0.00000000
C	28.39874584	-13.52236001	0.00000000
C	28.42858819	-12.12144910	0.00000000
C	28.38378991	-9.27136104	0.00000000
C	28.39951410	-7.87660534	0.00000000
C	28.39949388	7.87663459	0.00000000
C	28.38376632	9.27138911	0.00000000
C	28.42855838	12.12147503	0.00000000
C	28.39871354	13.52238530	0.00000000
C	29.62236139	-11.39400840	0.00000000
C	29.64763847	-9.99177480	0.00000000
C	29.59269114	-7.14264022	0.00000000
C	29.60299680	-5.74755806	0.00000000
C	29.60298114	5.74759208	0.00000000
C	29.59267173	7.14267306	0.00000000
C	29.64761181	9.99180469	0.00000000
C	29.62233178	11.39403701	0.00000000
C	30.83847937	-9.26114812	0.00000000
C	30.85840536	-7.85802268	0.00000000
C	30.79347948	-5.01110488	0.00000000
C	30.79923869	-3.61270829	0.00000000

C	30.79922813	3.61274732	0.00000000
C	30.79346483	5.01114299	0.00000000
C	30.85838242	7.85805778	0.00000000
C	30.83845287	9.26118146	0.00000000
C	32.04699373	-7.12311426	0.00000000
C	32.06013520	-5.72088582	0.00000000
C	31.98547372	-2.87871298	0.00000000
C	31.98672083	-1.47178196	0.00000000
C	31.98671589	1.47182553	0.00000000
C	31.98546448	2.87875611	0.00000000
C	32.06011698	5.72092682	0.00000000
C	32.04697133	7.12315347	0.00000000
C	33.24805583	-4.97862693	0.00000000
C	33.24819273	-3.58154751	0.00000000
C	33.15111930	-0.72552731	0.00000000
C	33.15111664	0.72557515	0.00000000
C	33.24818038	3.58159419	0.00000000
C	33.24803882	4.97867228	0.00000000
C	34.42814802	-2.81512282	0.00000000
C	34.41131859	-1.42878374	0.00000000
C	34.41131361	1.42883541	0.00000000
C	34.42813778	2.81517393	0.00000000
C	35.62692528	-0.67999386	0.00000000
C	35.62692274	0.68004975	0.00000000
H	-36.57287028	-1.23898534	0.00000000
H	-36.57286662	1.23901518	0.00000000
H	-35.39776236	-3.33508859	0.00000000
H	-35.39775212	3.33511451	0.00000000
H	-34.20958234	-5.51312889	0.00000000
H	-34.20956607	5.51314985	0.00000000
H	-33.00573805	-7.66264921	0.00000000
H	-33.00571670	7.66266579	0.00000000
H	-31.79517722	-9.80436172	0.00000000
H	-31.79515187	9.80437486	0.00000000
H	-31.00828459	-0.97161543	0.00000000
H	-31.00828242	0.97162895	0.00000000
H	-30.57706932	-11.94076352	0.00000000
H	-30.57704075	11.94077499	0.00000000
H	-29.83857103	-3.07645456	0.00000000
H	-29.83856389	3.07646552	0.00000000
H	-29.35152295	-14.07250780	0.00000000
H	-29.35149131	14.07251934	0.00000000
H	-28.64452869	-5.20761239	0.00000000
H	-28.64451652	5.20762039	0.00000000
H	-28.11871477	-16.19986532	0.00000000
H	-28.11867993	16.19987781	0.00000000
H	-27.44294724	-7.33326470	0.00000000
H	-27.44292976	7.33327054	0.00000000
H	-26.87887605	-18.32288387	0.00000000
H	-26.87883832	18.32289664	0.00000000
H	-26.23413255	-9.45421377	0.00000000
H	-26.23410943	9.45421848	0.00000000
H	-25.63219443	-20.44159265	0.00000000
H	-25.63215531	20.44160355	0.00000000
H	-25.01775819	-11.57080523	0.00000000
H	-25.01772918	11.57080998	0.00000000
H	-24.37868149	-22.55618294	0.00000000
H	-24.37864340	22.55618960	0.00000000
H	-23.79376225	-13.68323671	0.00000000
H	-23.79372761	13.68324248	0.00000000
H	-23.11803995	-24.66709284	0.00000000
H	-23.11800486	24.66709438	0.00000000
H	-22.56230051	-15.79155059	0.00000000
H	-22.56226155	15.79155753	0.00000000
H	-21.84879747	-26.77648593	0.00000000
H	-21.84876556	26.77648300	0.00000000
H	-21.32359972	-17.89582928	0.00000000
H	-21.32355885	17.89583619	0.00000000
H	-20.54951955	-28.88670006	0.00000000
H	-20.54948877	28.88669451	0.00000000
H	-20.07785679	-19.99641646	0.00000000
H	-20.07781682	19.99642111	0.00000000
H	-19.31697790	-30.94645166	0.00000000
H	-19.31694431	30.94644445	0.00000000
H	-18.82526385	-22.09395216	0.00000000
H	-18.82522680	22.09395244	0.00000000
H	-17.56532895	-24.18872314	0.00000000
H	-17.56529499	24.18871807	0.00000000
H	-17.16712751	-32.17987118	0.00000000
H	-17.16709597	32.17985952	0.00000000
H	-16.31722062	-26.25114392	0.00000000
H	-16.31718773	26.25113431	0.00000000
H	-14.76695607	-32.20403242	0.00000000

H	-14.62841529	-27.22039598	0.00000000
H	-14.62839133	27.22037750	0.00000000
H	-14.76692518	32.20401932	0.00000000
H	-12.28933090	-32.26051937	0.00000000
H	-12.21801557	-27.25650718	0.00000000
H	-12.21799507	27.25648395	0.00000000
H	-12.28930263	32.26050314	0.00000000
H	-9.82815456	-32.29151110	0.00000000
H	-9.77337474	-27.28686799	0.00000000
H	-9.77335803	27.28683996	0.00000000
H	-9.82813080	32.29149209	0.00000000
H	-7.37042896	-32.31494183	0.00000000
H	-7.32963647	-27.31009170	0.00000000
H	-7.32962299	27.31005966	0.00000000
H	-7.37040948	32.31492067	0.00000000
H	-4.91348870	-32.33134909	0.00000000
H	-4.88639405	-27.32684204	0.00000000
H	-4.88638290	27.32680712	0.00000000
H	-4.91347305	32.33132604	0.00000000
H	-2.45674904	-32.34108616	0.00000000
H	-2.44323448	-27.33694253	0.00000000
H	-2.44322496	27.33690572	0.00000000
H	-2.45673657	32.34106147	0.00000000
H	0.00000279	-32.34431616	0.00000000
H	0.00000281	-27.34031526	0.00000000
H	0.00001110	27.34027745	0.00000000
H	0.00001246	32.34429031	0.00000000
H	2.45675399	-32.34108598	0.00000000
H	2.44323945	-27.33694276	0.00000000
H	2.44324643	27.33690488	0.00000000
H	2.45676073	32.34105966	0.00000000
H	4.91349183	-32.33134876	0.00000000
H	4.88639716	-27.32684244	0.00000000
H	4.88640227	27.32680539	0.00000000
H	4.91349507	32.33132254	0.00000000
H	7.37042959	-32.31494141	0.00000000
H	7.32963701	-27.31009217	0.00000000
H	7.32963938	27.31005692	0.00000000
H	7.37042844	32.31491566	0.00000000
H	9.82815259	-32.29151064	0.00000000
H	9.77337260	-27.28686844	0.00000000
H	9.77337111	27.28683612	0.00000000
H	9.82814637	32.29148577	0.00000000
H	12.28932674	-32.26051887	0.00000000
H	12.21801116	-27.25650752	0.00000000
H	12.21800501	27.25647897	0.00000000
H	12.28931505	32.26049561	0.00000000
H	14.76695029	-32.20403179	0.00000000
H	14.62840921	-27.22039613	0.00000000
H	14.62839859	27.22037126	0.00000000
H	14.76693473	32.20401045	0.00000000
H	16.31721336	-26.25114459	0.00000000
H	16.31719268	26.25112903	0.00000000
H	17.16712048	-32.17987069	0.00000000
H	17.16710254	32.17985013	0.00000000
H	17.56532154	-24.18872425	0.00000000
H	17.56529891	24.18871529	0.00000000
H	18.82525626	-22.09395346	0.00000000
H	18.82522922	22.09395259	0.00000000
H	19.31697032	-30.94645162	0.00000000
H	19.31694910	30.94643535	0.00000000
H	20.07784913	-19.99641754	0.00000000
H	20.07781754	19.99642442	0.00000000
H	20.54951176	-28.88670060	0.00000000
H	20.54949136	28.88668756	0.00000000
H	21.32359208	-17.89582966	0.00000000
H	21.32355777	17.89584260	0.00000000
H	21.84878961	-26.77648689	0.00000000
H	21.84876655	26.77647855	0.00000000
H	22.56229305	-15.79154978	0.00000000
H	22.56225879	15.79156665	0.00000000
H	23.11803210	-24.66709396	0.00000000
H	23.11800402	24.66709264	0.00000000
H	23.79375515	-13.68323427	0.00000000
H	23.79372348	13.68325368	0.00000000
H	24.37867386	-22.55618395	0.00000000
H	24.37864061	22.55619104	0.00000000
H	25.01775165	-11.57080085	0.00000000
H	25.01772415	11.57082253	0.00000000
H	25.63218735	-20.44159323	0.00000000
H	25.63215079	20.44160833	0.00000000
H	26.23412674	-9.45420731	0.00000000
H	26.23410404	9.45423171	0.00000000

H	26.87886984	-18.32288362	0.00000000
H	26.87883254	18.32290460	0.00000000
H	27.44294230	-7.33325621	0.00000000
H	27.44292452	7.33328395	0.00000000
H	28.11870969	-16.19986382	0.00000000
H	28.11867346	16.19988847	0.00000000
H	28.64452465	-5.20760211	0.00000000
H	28.64451186	5.20763367	0.00000000
H	29.35151911	-14.07250467	0.00000000
H	29.35148471	14.07253204	0.00000000
H	29.83856785	-3.07644276	0.00000000
H	29.83856013	3.07647853	0.00000000
H	30.57706668	-11.94075846	0.00000000
H	30.57703450	11.94078903	0.00000000
H	31.00828223	-0.97160251	0.00000000
H	31.00827984	0.97164157	0.00000000
H	31.79517557	-9.80435459	0.00000000
H	31.79514632	9.80438964	0.00000000
H	33.00573710	-7.66264008	0.00000000
H	33.00571205	7.66268089	0.00000000
H	34.20958175	-5.51311808	0.00000000
H	34.20956246	5.51316513	0.00000000
H	35.39776216	-3.33507627	0.00000000
H	35.39774986	3.33512976	0.00000000
H	36.57287001	-1.23897119	0.00000000
H	36.57286559	1.23902970	0.00000000

Cartesian coordinates (in Å) for the lowest triplet states of n -HGQRs ($n = 3$ –15), calculated by spin-unrestricted TAO-LDA.

3-HGQR (triplet)

C	-6.14982306	-0.68663278	0.00000000
C	-6.14982308	0.68663274	0.00000000
C	-4.90915205	-2.83459886	0.00000000
C	-4.93905696	-1.43288232	0.00000000
C	-4.93905703	1.43288239	0.00000000
C	-4.90915218	2.83459893	0.00000000
C	-3.66975112	-4.98350923	0.00000000
C	-3.71052289	-3.56172195	0.00000000
C	-3.69813986	-0.72017989	0.00000000
C	-3.69813989	0.72018007	0.00000000
C	-3.71052301	3.56172203	0.00000000
C	-3.66975124	4.98350938	0.00000000
C	-2.48057993	-5.67023351	0.00000000
C	-2.47285770	-2.84346777	0.00000000
C	-2.51470237	-1.45238588	0.00000000
C	-2.51470249	1.45238606	0.00000000
C	-2.47285782	2.84346785	0.00000000
C	-2.48057998	5.67023365	0.00000000
C	-1.22889468	-4.99484708	0.00000000
C	-1.22563148	-3.56369226	0.00000000
C	-1.22563164	3.56369229	0.00000000
C	-1.22889472	4.99484713	0.00000000
C	0.00000001	-5.66959022	0.00000000
C	0.00000008	-2.90457827	0.00000000
C	-0.00000011	2.90457829	0.00000000
C	0.00000001	5.66959026	0.00000000
C	1.22889472	-4.99484708	0.00000000
C	1.22563164	-3.56369225	0.00000000
C	1.22563148	3.56369225	0.00000000
C	1.22889469	4.99484707	0.00000000
C	2.48057997	-5.67023361	0.00000000
C	2.47285783	-2.84346782	0.00000000
C	2.51470250	-1.45238603	0.00000000
C	2.51470239	1.45238588	0.00000000
C	2.47285770	2.84346776	0.00000000
C	2.48057993	5.67023347	0.00000000
C	3.66975123	-4.98350935	0.00000000
C	3.71052300	-3.56172201	0.00000000
C	3.69813991	-0.72018007	0.00000000
C	3.69813988	0.72017989	0.00000000
C	3.71052289	3.56172193	0.00000000
C	3.66975113	4.98350921	0.00000000
C	4.90915218	-2.83459893	0.00000000
C	4.93905703	-1.43288241	0.00000000
C	4.93905697	1.43288231	0.00000000
C	4.90915205	2.83459883	0.00000000
C	6.14982309	-0.68663278	0.00000000
C	6.14982305	0.68663273	0.00000000
H	-7.09975392	-1.23864117	0.00000000
H	-7.09975401	1.23864108	0.00000000
H	-5.86205336	-3.38464067	0.00000000
H	-5.86205351	3.38464073	0.00000000
H	-4.62276553	-5.53019395	0.00000000
H	-4.62276566	5.53019415	0.00000000
H	-2.47748406	-6.76889749	0.00000000
H	-2.47748410	6.76889765	0.00000000
H	-1.56673530	-0.90567733	0.00000000
H	-1.56673543	0.90567751	0.00000000
H	0.00000003	-6.76983452	0.00000000
H	0.00000007	-1.81027039	0.00000000
H	-0.00000014	1.81027041	0.00000000
H	0.00000002	6.76983455	0.00000000
H	1.56673544	-0.90567747	0.00000000
H	1.56673533	0.90567732	0.00000000
H	2.47748407	-6.76889761	0.00000000
H	2.47748408	6.76889745	0.00000000
H	4.62276564	-5.53019413	0.00000000
H	4.62276554	5.53019393	0.00000000
H	5.86205351	-3.38464074	0.00000000
H	5.86205334	3.38464065	0.00000000
H	7.09975400	-1.23864110	0.00000000
H	7.09975393	1.23864111	0.00000000

4-HGQR (triplet)

C	-8.59866514	-0.68298084	0.00000000
C	-8.59866502	0.68298185	0.00000000
C	-7.38612152	-2.82945633	0.00000000
C	-7.38613360	-1.43387689	0.00000000
C	-7.38613336	1.43387768	0.00000000

C	-7.38612115	2.82945705	0.00000000
C	-6.14332343	-4.98237197	0.00000000
C	-6.19595715	-3.57754371	0.00000000
C	-6.13710463	-0.72274582	0.00000000
C	-6.13710453	0.72274644	0.00000000
C	-6.19595681	3.57754423	0.00000000
C	-6.14332286	4.98237231	0.00000000
C	-4.89074652	-7.10558005	0.00000000
C	-4.93468765	-5.67998096	0.00000000
C	-4.95166390	-2.85907458	0.00000000
C	-4.96241364	-1.45895401	0.00000000
C	-4.96241351	1.45895448	0.00000000
C	-4.95166373	2.85907498	0.00000000
C	-4.93468711	5.67998099	0.00000000
C	-4.89074590	7.10557988	0.00000000
C	-3.70792793	-7.78866469	0.00000000
C	-3.69434172	-4.95372022	0.00000000
C	-3.74441569	-3.56817408	0.00000000
C	-3.74441550	3.56817419	0.00000000
C	-3.69434140	4.95372018	0.00000000
C	-3.70792737	7.78866430	0.00000000
C	-2.45139211	-7.11401920	0.00000000
C	-2.44269801	-5.67658548	0.00000000
C	-2.44269775	5.67658520	0.00000000
C	-2.45139181	7.11401876	0.00000000
C	-1.24291558	-7.81190652	0.00000000
C	-1.21778702	-5.02739645	0.00000000
C	-1.21778702	5.02739610	0.00000000
C	-1.24291545	7.81190593	0.00000000
C	-0.00000003	-7.15521051	0.00000000
C	0.00000002	-5.71821612	0.00000000
C	-0.00000014	5.71821568	0.00000000
C	-0.00000016	7.15520991	0.00000000
C	1.24291545	-7.81190665	0.00000000
C	1.21778712	-5.02739654	0.00000000
C	1.21778676	5.02739611	0.00000000
C	1.24291516	7.81190592	0.00000000
C	2.45139204	-7.11401942	0.00000000
C	2.44269806	-5.67658568	0.00000000
C	2.44269753	5.67658520	0.00000000
C	2.45139156	7.11401878	0.00000000
C	3.70792785	-7.78866495	0.00000000
C	3.69434182	-4.95372050	0.00000000
C	3.74441588	-3.56817433	0.00000000
C	3.74441534	3.56817413	0.00000000
C	3.69434121	4.95372017	0.00000000
C	3.70792713	7.78866440	0.00000000
C	4.89074650	-7.10558037	0.00000000
C	4.93468775	-5.67998128	0.00000000
C	4.95166416	-2.85907488	0.00000000
C	4.96241383	-1.45895425	0.00000000
C	4.96241354	1.45895434	0.00000000
C	4.95166360	2.85907488	0.00000000
C	4.93468694	5.67998103	0.00000000
C	4.89074570	7.10557999	0.00000000
C	6.14332361	-4.98237235	0.00000000
C	6.19595744	-3.57754407	0.00000000
C	6.13710481	-0.72274596	0.00000000
C	6.13710467	0.72274635	0.00000000
C	6.19595670	3.57754417	0.00000000
C	6.14332275	4.98237232	0.00000000
C	7.38612179	-2.82945660	0.00000000
C	7.38613380	-1.43387709	0.00000000
C	7.38613353	1.43387764	0.00000000
C	7.38612118	2.82945705	0.00000000
C	8.59866537	-0.68298097	0.00000000
C	8.59866523	0.68298177	0.00000000
H	-9.54729826	-1.23736424	0.00000000
H	-9.54729804	1.23736537	0.00000000
H	-8.34992773	-3.35993023	0.00000000
H	-8.34992740	3.35993075	0.00000000
H	-7.08449508	-5.55209214	0.00000000
H	-7.08449435	5.55209262	0.00000000
H	-5.84520779	-7.64986444	0.00000000
H	-5.84520703	7.64986435	0.00000000
H	-3.98812979	-0.95213024	0.00000000
H	-3.98812973	0.95213060	0.00000000
H	-3.70212902	-8.88738533	0.00000000
H	-3.70212841	8.88738484	0.00000000
H	-2.81835423	-2.97774407	0.00000000
H	-2.81835422	2.97774402	0.00000000
H	-1.26559938	-8.91181611	0.00000000
H	-1.16978014	-3.93024373	0.00000000

H	-1.16978023	3.93024345	0.00000000
H	-1.26559922	8.91181541	0.00000000
H	1.26559921	-8.91181624	0.00000000
H	1.16978033	-3.93024380	0.00000000
H	1.16978000	3.93024346	0.00000000
H	1.26559890	8.91181540	0.00000000
H	2.81835446	-2.97774421	0.00000000
H	2.81835404	2.97774397	0.00000000
H	3.70212895	-8.88738560	0.00000000
H	3.70212809	8.88738496	0.00000000
H	3.98812993	-0.95213053	0.00000000
H	3.98812981	0.95213035	0.00000000
H	5.84520773	-7.64986487	0.00000000
H	5.84520686	7.64986444	0.00000000
H	7.08449523	-5.55209263	0.00000000
H	7.08449428	5.55209261	0.00000000
H	8.34992818	-3.35993023	0.00000000
H	8.34992729	3.35993109	0.00000000
H	9.54729853	-1.23736437	0.00000000
H	9.54729828	1.23736531	0.00000000

5-HGQR (triplet)

C	-11.04918206	-0.68123796	0.00000000
C	-11.04918183	0.68124209	0.00000000
C	-9.84194142	-2.82392429	0.00000000
C	-9.83495372	-1.43351249	0.00000000
C	-9.83495343	1.43351628	0.00000000
C	-9.84194092	2.82392756	0.00000000
C	-8.63250445	-4.98413267	0.00000000
C	-8.65554199	-3.58296191	0.00000000
C	-8.58151756	-0.72449356	0.00000000
C	-8.58151749	0.72449737	0.00000000
C	-8.65554187	3.58296465	0.00000000
C	-8.63250443	4.98413460	0.00000000
C	-7.36611072	-7.11115910	0.00000000
C	-7.43035168	-5.70417246	0.00000000
C	-7.40262791	-2.86650220	0.00000000
C	-7.41194139	-1.46234007	0.00000000
C	-7.41194145	1.46234347	0.00000000
C	-7.40262826	2.86650515	0.00000000
C	-7.43035225	5.70417372	0.00000000
C	-7.36611141	7.11115953	0.00000000
C	-6.11403953	-9.22766459	0.00000000
C	-6.15836087	-7.79993419	0.00000000
C	-6.18360747	-4.97694444	0.00000000
C	-6.20565733	-3.58234811	0.00000000
C	-6.20565817	3.58235052	0.00000000
C	-6.18360862	4.97694610	0.00000000
C	-6.15836228	7.79993419	0.00000000
C	-6.11404134	9.22766399	0.00000000
C	-4.93420596	-9.90892385	0.00000000
C	-4.91772340	-7.06861376	0.00000000
C	-4.97201395	-5.68667509	0.00000000
C	-4.97201559	5.68667606	0.00000000
C	-4.91772540	7.06861398	0.00000000
C	-4.93420834	9.90892318	0.00000000
C	-3.67571165	-9.23337488	0.00000000
C	-3.66298874	-7.79316255	0.00000000
C	-3.66299129	7.79316258	0.00000000
C	-3.67571449	9.23337441	0.00000000
C	-2.47525601	-9.93478258	0.00000000
C	-2.43914027	-7.14932694	0.00000000
C	-2.43914326	7.14932722	0.00000000
C	-2.47525937	9.93478218	0.00000000
C	-1.22471004	-9.28693335	0.00000000
C	-1.21856977	-7.84346837	0.00000000
C	-1.21857320	7.84346865	0.00000000
C	-1.22471357	9.28693334	0.00000000
C	0.00000264	-9.96782498	0.00000000
C	0.00000217	-7.16499915	0.00000000
C	-0.00000138	7.16499955	0.00000000
C	-0.00000116	9.96782514	0.00000000
C	1.22471494	-9.28693275	0.00000000
C	1.21857422	-7.84346797	0.00000000
C	1.21857062	7.84346840	0.00000000
C	1.22471124	9.28693323	0.00000000
C	2.47526094	-9.93478126	0.00000000
C	2.43914411	-7.14932627	0.00000000
C	2.43914077	7.14932666	0.00000000
C	2.47525727	9.93478201	0.00000000
C	3.67571581	-9.23337308	0.00000000
C	3.66299220	-7.79316134	0.00000000
C	3.66298929	7.79316185	0.00000000
C	3.67571257	9.23337404	0.00000000

C	4.93420970	-9.90892150	0.00000000
C	4.91772595	-7.06861251	0.00000000
C	4.97201563	-5.68667490	0.00000000
C	4.97201407	5.68667427	0.00000000
C	4.91772372	7.06861281	0.00000000
C	4.93420689	9.90892272	0.00000000
C	6.11404232	-9.22766201	0.00000000
C	6.15836273	-7.79993241	0.00000000
C	6.18360836	-4.97694505	0.00000000
C	6.20565758	-3.58234989	0.00000000
C	6.20565697	3.58234733	0.00000000
C	6.18360734	4.97694351	0.00000000
C	6.15836121	7.79993299	0.00000000
C	6.11404020	9.22766327	0.00000000
C	7.36611137	-7.11115774	0.00000000
C	7.43035181	-5.70417234	0.00000000
C	7.40262734	-2.86650479	0.00000000
C	7.41194030	-1.46234351	0.00000000
C	7.41194044	1.46233939	0.00000000
C	7.40262725	2.86650130	0.00000000
C	7.43035154	5.70417123	0.00000000
C	7.36611083	7.11115776	0.00000000
C	8.63250354	-4.98413347	0.00000000
C	8.65554066	-3.58296403	0.00000000
C	8.58151608	-0.72449776	0.00000000
C	8.58151628	0.72449290	0.00000000
C	8.65554128	3.58296073	0.00000000
C	8.63250407	4.98413134	0.00000000
C	9.84193932	-2.82392724	0.00000000
C	9.83495178	-1.43351645	0.00000000
C	9.83495237	1.43351145	0.00000000
C	9.84194039	2.82392299	0.00000000
C	11.04918006	-0.68124270	0.00000000
C	11.04918046	0.68123703	0.00000000
H	-11.99698028	-1.23710314	0.00000000
H	-11.99697992	1.23710723	0.00000000
H	-10.80828945	-3.34987642	0.00000000
H	-10.80828872	3.34987946	0.00000000
H	-9.58493978	-5.53453504	0.00000000
H	-9.58493941	5.53453674	0.00000000
H	-8.30459919	-7.68539542	0.00000000
H	-8.30459951	7.68539567	0.00000000
H	-7.06935274	-9.77049929	0.00000000
H	-7.06935432	9.77049846	0.00000000
H	-6.43603344	-0.95827768	0.00000000
H	-6.43603373	0.95828077	0.00000000
H	-5.25302134	-3.03188146	0.00000000
H	-5.25302247	3.03188392	0.00000000
H	-4.92660609	-11.00765700	0.00000000
H	-4.92660849	11.00765611	0.00000000
H	-4.04763335	-5.09332673	0.00000000
H	-4.04763522	5.09332796	0.00000000
H	-2.50315363	-11.03463062	0.00000000
H	-2.38770235	-6.05215890	0.00000000
H	-2.38770503	6.05215945	0.00000000
H	-2.50315708	11.03463005	0.00000000
H	0.00000281	-11.06783824	0.00000000
H	0.00000184	-6.06479855	0.00000000
H	-0.00000141	6.06479899	0.00000000
H	-0.00000112	11.06783831	0.00000000
H	2.50315890	-11.03462916	0.00000000
H	2.38770554	-6.05215855	0.00000000
H	2.38770249	6.05215874	0.00000000
H	2.50315523	11.03462993	0.00000000
H	4.04763512	-5.09332717	0.00000000
H	4.04763350	5.09332612	0.00000000
H	4.92661005	-11.00765441	0.00000000
H	4.92660728	11.00765577	0.00000000
H	5.25302198	-3.03188351	0.00000000
H	5.25302100	3.03188095	0.00000000
H	6.43603278	-0.95828085	0.00000000
H	6.43603255	0.95827727	0.00000000
H	7.06935533	-9.77049616	0.00000000
H	7.06935346	9.77049773	0.00000000
H	8.30459937	-7.68539365	0.00000000
H	8.30459931	7.68539386	0.00000000
H	9.58493836	-5.53453539	0.00000000
H	9.58493940	5.53453348	0.00000000
H	10.80828693	-3.34987900	0.00000000
H	10.80828840	3.34987489	0.00000000
H	11.99697791	-1.23710786	0.00000000
H	11.99697858	1.23710210	0.00000000

6-HGQR (triplet)

C	-13.49915371	-0.68054052	0.00000000
C	-13.49915430	0.68053414	0.00000000
C	-12.29551731	-2.82075520	0.00000000
C	-12.28454162	-1.43326805	0.00000000
C	-12.28454278	1.43326271	0.00000000
C	-12.29551957	2.82075012	0.00000000
C	-11.09572552	-4.98172126	0.00000000
C	-11.11051380	-3.58412449	0.00000000
C	-11.02777254	-0.72534202	0.00000000
C	-11.02777311	0.72533753	0.00000000
C	-11.11051643	3.58412057	0.00000000
C	-11.09572902	4.98171784	0.00000000
C	-9.86183726	-7.11728529	0.00000000
C	-9.89764688	-5.71371231	0.00000000
C	-9.85362122	-2.87099411	0.00000000
C	-9.86123121	-1.46461697	0.00000000
C	-9.86123223	1.46461352	0.00000000
C	-9.85362310	2.87099090	0.00000000
C	-9.89765054	5.71371015	0.00000000
C	-9.86184169	7.11728377	0.00000000
C	-8.58954588	-9.23592878	0.00000000
C	-8.65847811	-7.82803515	0.00000000
C	-8.64167618	-4.98805232	0.00000000
C	-8.66133626	-3.58983949	0.00000000
C	-8.66133833	3.58983741	0.00000000
C	-8.64167902	4.98805073	0.00000000
C	-8.65848257	7.82803496	0.00000000
C	-8.58955107	9.23592931	0.00000000
C	-7.33759536	-11.34781631	0.00000000
C	-7.38221787	-9.91954802	0.00000000
C	-7.41281000	-7.09539273	0.00000000
C	-7.44017796	-5.70334616	0.00000000
C	-7.44018085	5.70334574	0.00000000
C	-7.41281358	7.09539296	0.00000000
C	-7.38222289	9.91954972	0.00000000
C	-7.33760062	11.34781867	0.00000000
C	-6.15892190	-12.02823624	0.00000000
C	-6.14096749	-9.18456517	0.00000000
C	-6.19828939	-7.80453453	0.00000000
C	-6.19829294	7.80453596	0.00000000
C	-6.14097154	9.18456737	0.00000000
C	-6.15892683	12.02823944	0.00000000
C	-4.89995108	-11.35240499	0.00000000
C	-4.88467688	-9.90983485	0.00000000
C	-4.88468068	9.90983783	0.00000000
C	-4.89995499	11.35240863	0.00000000
C	-3.70403041	-12.05577873	0.00000000
C	-3.66108000	-9.26933825	0.00000000
C	-3.66108278	9.26934130	0.00000000
C	-3.70403356	12.05578296	0.00000000
C	-2.45046498	-11.41129613	0.00000000
C	-2.43941125	-9.96605775	0.00000000
C	-2.43941324	9.96606109	0.00000000
C	-2.45046714	11.41130025	0.00000000
C	-1.23308364	-12.09767152	0.00000000
C	-1.22048004	-9.29327728	0.00000000
C	-1.22048103	9.29328043	0.00000000
C	-1.23308475	12.09767591	0.00000000
C	-0.00000030	-11.42644439	0.00000000
C	-0.00000020	-9.97574044	0.00000000
C	-0.00000025	9.97574383	0.00000000
C	-0.00000032	11.42644857	0.00000000
C	1.23308297	-12.09767167	0.00000000
C	1.22047972	-9.29327746	0.00000000
C	1.22048060	9.29328057	0.00000000
C	1.23308404	12.09767602	0.00000000
C	2.45046441	-11.41129643	0.00000000
C	2.43941086	-9.96605806	0.00000000
C	2.43941277	9.96606136	0.00000000
C	2.45046653	11.41130050	0.00000000
C	3.70402981	-12.05577915	0.00000000
C	3.66107971	-9.26933872	0.00000000
C	3.66108238	9.26934170	0.00000000
C	3.70403293	12.05578329	0.00000000
C	4.89995061	-11.35240554	0.00000000
C	4.88467657	-9.90983539	0.00000000
C	4.88468031	9.90983824	0.00000000
C	4.89995447	11.35240906	0.00000000
C	6.15892137	-12.02823695	0.00000000
C	6.14096733	-9.18456579	0.00000000
C	6.19828947	-7.80453514	0.00000000
C	6.19829300	7.80453644	0.00000000
C	6.14097133	9.18456786	0.00000000

C	6.15892625	12.02824001	0.00000000
C	7.33759493	-11.34781713	0.00000000
C	7.38221764	-9.91954879	0.00000000
C	7.41281018	-7.09539338	0.00000000
C	7.44017833	-5.70334678	0.00000000
C	7.44018123	5.70334629	0.00000000
C	7.41281375	7.09539353	0.00000000
C	7.38222260	9.91955036	0.00000000
C	7.33760013	11.34781935	0.00000000
C	8.58954574	-9.23592960	0.00000000
C	8.65847822	-7.82803589	0.00000000
C	8.64167659	-4.98805289	0.00000000
C	8.66133683	-3.58984000	0.00000000
C	8.66133891	3.58983790	0.00000000
C	8.64167944	4.98805125	0.00000000
C	8.65848265	7.82803562	0.00000000
C	8.58955087	9.23593003	0.00000000
C	9.86183743	-7.11728600	0.00000000
C	9.89764724	-5.71371291	0.00000000
C	9.85362178	-2.87099451	0.00000000
C	9.86123181	-1.46461732	0.00000000
C	9.86123282	1.46461386	0.00000000
C	9.85362367	2.87099129	0.00000000
C	9.89765090	5.71371072	0.00000000
C	9.86184183	7.11728443	0.00000000
C	11.09572593	-4.98172172	0.00000000
C	11.11051434	-3.58412488	0.00000000
C	11.02777304	-0.72534211	0.00000000
C	11.02777361	0.72533764	0.00000000
C	11.11051695	3.58412094	0.00000000
C	11.09572942	4.98171828	0.00000000
C	12.29551782	-2.82075536	0.00000000
C	12.28454217	-1.43326813	0.00000000
C	12.28454332	1.43326281	0.00000000
C	12.29552007	2.82075030	0.00000000
C	13.49915430	-0.68054052	0.00000000
C	13.49915488	0.68053419	0.00000000
H	-14.44654259	-1.23711700	0.00000000
H	-14.44654365	1.23710998	0.00000000
H	-13.26303824	-3.34457574	0.00000000
H	-13.26304101	3.34457011	0.00000000
H	-12.05141847	-5.52650349	0.00000000
H	-12.05142256	5.52649961	0.00000000
H	-10.81090174	-7.67353317	0.00000000
H	-10.81090683	7.67353120	0.00000000
H	-9.52669275	-9.81237519	0.00000000
H	-9.52669859	9.81237535	0.00000000
H	-8.88433152	-0.96208725	0.00000000
H	-8.88433202	0.96208466	0.00000000
H	-8.29328267	-11.89000057	0.00000000
H	-8.29328838	11.89000286	0.00000000
H	-7.70626907	-3.04379682	0.00000000
H	-7.70627049	3.04379540	0.00000000
H	-6.49031278	-5.14833086	0.00000000
H	-6.49031495	5.14833093	0.00000000
H	-6.15034806	-13.12696696	0.00000000
H	-6.15035349	13.12697059	0.00000000
H	-5.27486393	-7.20937720	0.00000000
H	-5.27486674	7.20937890	0.00000000
H	-3.73432771	-13.15557777	0.00000000
H	-3.60777071	-8.17208148	0.00000000
H	-3.60777311	8.17208403	0.00000000
H	-3.73433095	13.15558251	0.00000000
H	-1.23970632	-13.19769200	0.00000000
H	-1.21522023	-8.19318287	0.00000000
H	-1.21522115	8.19318543	0.00000000
H	-1.23970739	13.19769697	0.00000000
H	1.23970550	-13.19769215	0.00000000
H	1.21522000	-8.19318305	0.00000000
H	1.21522080	8.19318559	0.00000000
H	1.23970656	13.19769709	0.00000000
H	3.73432696	-13.15557818	0.00000000
H	3.60777044	-8.17208199	0.00000000
H	3.60777269	8.17208447	0.00000000
H	3.73433020	13.15558283	0.00000000
H	5.27486409	-7.20937776	0.00000000
H	5.27486692	7.20937931	0.00000000
H	6.15034737	-13.12696767	0.00000000
H	6.15035276	13.12697115	0.00000000
H	6.49031320	-5.14833148	0.00000000
H	6.49031539	5.14833148	0.00000000
H	7.70626970	-3.04379734	0.00000000
H	7.70627115	3.04379589	0.00000000

H	8.29328216	-11.89000151	0.00000000
H	8.29328779	11.89000366	0.00000000
H	8.88433213	-0.96208775	0.00000000
H	8.88433264	0.96208516	0.00000000
H	9.52669249	-9.81237614	0.00000000
H	9.52669826	9.81237622	0.00000000
H	10.81090181	-7.67353395	0.00000000
H	10.81090686	7.67353195	0.00000000
H	12.05141885	-5.52650391	0.00000000
H	12.05142292	5.52650001	0.00000000
H	13.26303876	-3.34457581	0.00000000
H	13.26304151	3.34457021	0.00000000
H	14.44654315	-1.23711700	0.00000000
H	14.44654420	1.23711003	0.00000000

7-HGQR (triplet)

C	-15.95006779	-0.68039520	0.00000000
C	-15.95006832	0.68038863	0.00000000
C	-14.74842494	-2.81899230	0.00000000
C	-14.73551676	-1.43254159	0.00000000
C	-14.73551787	1.43253594	0.00000000
C	-14.74842695	2.81898681	0.00000000
C	-13.55456381	-4.98044631	0.00000000
C	-13.56468124	-3.58422959	0.00000000
C	-13.47699018	-0.72543942	0.00000000
C	-13.47699069	0.72543457	0.00000000
C	-13.56468360	3.58422507	0.00000000
C	-13.55456692	4.98044211	0.00000000
C	-12.33058067	-7.11767638	0.00000000
C	-12.35864429	-5.71690654	0.00000000
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H	-10.74254248	16.12878787	0.00000000
H	-10.18874523	-7.28163945	0.00000000
H	-10.18874949	7.28163791	0.00000000
H	-8.95596194	-9.38206946	0.00000000
H	-8.95596653	9.38207310	0.00000000
H	-8.59773727	-17.36586282	0.00000000
H	-8.59774502	17.36587456	0.00000000
H	-7.72852670	-11.44413245	0.00000000
H	-7.72853205	11.44414030	0.00000000
H	-6.18900058	-17.39488265	0.00000000
H	-6.05269912	-12.41110455	0.00000000
H	-6.05270276	12.41111605	0.00000000
H	-6.18900642	17.39489502	0.00000000
H	-3.70228263	-17.44562670	0.00000000
H	-3.65320268	-12.44053442	0.00000000
H	-3.65320475	12.44054755	0.00000000
H	-3.70228658	17.44563975	0.00000000
H	-1.23315641	-17.46180278	0.00000000
H	-1.21758489	-12.45569579	0.00000000
H	-1.21758577	12.45570982	0.00000000
H	-1.23315787	17.46181617	0.00000000
H	1.23317357	-17.46180045	0.00000000
H	1.21759313	-12.45569375	0.00000000
H	1.21759350	12.45570781	0.00000000
H	1.23317454	17.46181384	0.00000000
H	3.70229922	-17.44561975	0.00000000
H	3.65321050	-12.44052836	0.00000000
H	3.65321198	12.44054154	0.00000000
H	3.70230284	17.44563269	0.00000000
H	6.18901602	-17.39487110	0.00000000
H	6.05270635	-12.41109462	0.00000000
H	6.05270902	12.41110603	0.00000000
H	6.18902168	17.39488308	0.00000000
H	7.72853073	-11.44412156	0.00000000
H	7.72853572	11.44412877	0.00000000
H	8.59775091	-17.36584730	0.00000000
H	8.59775862	17.36585821	0.00000000
H	8.95596269	-9.38205932	0.00000000
H	8.95596659	9.38206253	0.00000000
H	10.18874209	-7.28163130	0.00000000
H	10.18874555	7.28162914	0.00000000
H	10.74254399	-16.12875970	0.00000000
H	10.74255272	16.12876812	0.00000000
H	11.40763287	-5.17403347	0.00000000
H	11.40763602	5.17402563	0.00000000
H	11.97406647	-14.05842098	0.00000000
H	11.97407542	14.05842634	0.00000000
H	12.61302024	-3.05815021	0.00000000
H	12.61302274	3.05813740	0.00000000
H	13.26319930	-11.93152966	0.00000000
H	13.26320886	11.93153030	0.00000000
H	13.78696052	-0.96654324	0.00000000
H	13.78696169	0.96652704	0.00000000
H	14.51391528	-9.80211629	0.00000000
H	14.51392529	9.80211097	0.00000000
H	15.74895879	-7.66651468	0.00000000
H	15.74896869	7.66650297	0.00000000
H	16.97089728	-5.51993273	0.00000000
H	16.97090599	5.51991509	0.00000000
H	18.17116987	-3.34001008	0.00000000
H	18.17117610	3.33998772	0.00000000
H	19.35026950	-1.23791354	0.00000000
H	19.35027206	1.23788763	0.00000000
9-HGQR (triplet)			
C	-20.85876726	-0.68043739	0.00000000
C	-20.85876968	0.68042382	0.00000000
C	-19.65822576	-2.81750239	0.00000000
C	-19.64399309	-1.43050991	0.00000000
C	-19.64399847	1.43050067	0.00000000
C	-19.65823645	2.81749204	0.00000000
C	-18.47049095	-4.97980757	0.00000000
C	-18.47656603	-3.58263155	0.00000000
C	-18.38497025	-0.72511151	0.00000000
C	-18.38497318	0.72510753	0.00000000
C	-18.47658063	3.58262482	0.00000000
C	-18.47051154	4.97979883	0.00000000
C	-17.25732763	-7.12003066	0.00000000

C	-17.27869942	-5.71887134	0.00000000
C	-17.21573583	-2.87535272	0.00000000
C	-17.21961119	-1.46902363	0.00000000
C	-17.21961764	1.46902360	0.00000000
C	-17.21574875	2.87535161	0.00000000
C	-17.27872447	5.71886545	0.00000000
C	-17.25735897	7.12002208	0.00000000
C	-16.03244561	-9.25120108	0.00000000
C	-16.06254616	-7.85037635	0.00000000
C	-16.01504626	-5.00196001	0.00000000
C	-16.02714680	-3.60333668	0.00000000
C	-16.02716404	3.60333882	0.00000000
C	-16.01507017	5.00196003	0.00000000
C	-16.06258239	7.85037012	0.00000000
C	-16.03248827	9.25119201	0.00000000
C	-14.79521870	-11.37507585	0.00000000
C	-14.83295601	-9.97524561	0.00000000
C	-14.80130434	-7.12531571	0.00000000
C	-14.82128985	-5.72875568	0.00000000
C	-14.82131847	5.72875810	0.00000000
C	-14.80133969	7.12531539	0.00000000
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C	-14.79527250	11.37506715	0.00000000
C	-13.54474853	-13.49326585	0.00000000
C	-13.59116400	-12.09173389	0.00000000
C	-13.57581579	-9.24307759	0.00000000
C	-13.60392313	-7.84583605	0.00000000
C	-13.60396314	7.84583778	0.00000000
C	-13.57586227	9.24307668	0.00000000
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C	-13.54481232	13.49325968	0.00000000
C	-12.26354461	-15.60067530	0.00000000
C	-12.33671740	-14.19492826	0.00000000
C	-12.33976503	-11.35360872	0.00000000
C	-12.37499311	-9.95633474	0.00000000
C	-12.37504362	9.95633612	0.00000000
C	-12.33982146	11.35360836	0.00000000
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C	-11.13341485	12.06137114	0.00000000
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C	-11.01174978	17.70729613	0.00000000
C	-9.83285964	-18.38691641	0.00000000
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C	-9.87788056	-14.15979877	0.00000000
C	-9.87794647	14.15980569	0.00000000
C	-9.81493037	15.54113982	0.00000000
C	-9.83293714	18.38692964	0.00000000
C	-8.57658159	-17.70879801	0.00000000
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C	-8.55859631	16.26550756	0.00000000
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C	-7.38255600	-18.41432931	0.00000000
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C	-7.38262421	18.41435108	0.00000000
C	-6.12941392	-17.77323058	0.00000000
C	-6.11157898	-16.32751523	0.00000000
C	-6.11163766	16.32753272	0.00000000
C	-6.12947477	17.77325337	0.00000000
C	-4.91684497	-18.46689786	0.00000000
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C	-4.88658540	15.66244456	0.00000000
C	-4.91689880	18.46692424	0.00000000
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C	-3.66941865	16.35162529	0.00000000
C	-3.68094556	17.80461471	0.00000000
C	-2.45747459	-18.48745236	0.00000000
C	-2.44252309	-15.68192762	0.00000000
C	-2.44255556	15.68194608	0.00000000
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C	-1.22732062	-17.81867056	0.00000000
C	-1.22346623	-16.36369632	0.00000000
C	-1.22348832	16.36371696	0.00000000
C	-1.22734316	17.81869919	0.00000000
C	-0.00000949	-18.49423459	0.00000000
C	-0.00000534	-15.68819291	0.00000000

C	-0.00001625	15.68821177	0.00000000
C	-0.00002044	18.49426559	0.00000000
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C	1.22345392	16.36372059	0.00000000
C	1.22730452	17.81870306	0.00000000
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C	2.44252362	15.68195314	0.00000000
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C	6.11160670	16.32755082	0.00000000
C	6.12943961	17.77327264	0.00000000
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C	7.33162329	-15.62797734	0.00000000
C	7.33166689	15.62799190	0.00000000
C	7.38258836	18.41437474	0.00000000
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C	11.13340422	12.06139225	0.00000000
C	11.09487165	13.45483053	0.00000000
C	11.05459846	16.28029483	0.00000000
C	11.01172156	17.70732942	0.00000000
C	12.26354130	-15.60070963	0.00000000
C	12.33671715	-14.19496132	0.00000000
C	12.33977078	-11.35363769	0.00000000
C	12.37500190	-9.95636132	0.00000000
C	12.37504204	9.95635151	0.00000000
C	12.33981541	11.35362879	0.00000000
C	12.33677051	14.19495631	0.00000000
C	12.26359837	15.60070742	0.00000000
C	13.54475148	-13.49330006	0.00000000
C	13.59117012	-12.09176634	0.00000000
C	13.57582782	-9.24310500	0.00000000
C	13.60393793	-7.84586080	0.00000000
C	13.60397099	7.84584580	0.00000000
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C	14.82133544	5.72875834	0.00000000
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C	14.83300956	9.97525734	0.00000000
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C	16.02717322	-3.60335639	0.00000000
C	16.02718906	3.60333210	0.00000000
C	16.01509207	5.00195798	0.00000000
C	16.06259833	7.85038013	0.00000000
C	16.03249990	9.25120791	0.00000000
C	17.25735040	-7.12005907	0.00000000
C	17.27872492	-5.71889672	0.00000000
C	17.21576579	-2.87537226	0.00000000
C	17.21964349	-1.46904065	0.00000000
C	17.21964984	1.46901154	0.00000000
C	17.21577824	2.87534315	0.00000000
C	17.27874911	5.71886713	0.00000000

C	17.25738004	7.12002932	0.00000000
C	18.47051961	-4.97983298	0.00000000
C	18.47659751	-3.58265387	0.00000000
C	18.38500577	-0.72512740	0.00000000
C	18.38500885	0.72509359	0.00000000
C	18.47661272	3.58261942	0.00000000
C	18.47054053	4.97979824	0.00000000
C	19.65826052	-2.81752484	0.00000000
C	19.64402947	-1.43052914	0.00000000
C	19.64403565	1.43048986	0.00000000
C	19.65827237	2.81748532	0.00000000
C	20.85880547	-0.68045439	0.00000000
C	20.85880834	0.68040989	0.00000000
H	-21.80536026	-1.23830684	0.00000000
H	-21.80536470	1.23828933	0.00000000
H	-20.62702882	-3.33895781	0.00000000
H	-20.62704116	3.33894295	0.00000000
H	-19.42975951	-5.51831573	0.00000000
H	-19.42978142	5.51830226	0.00000000
H	-18.21265146	-7.66553681	0.00000000
H	-18.21268375	7.66552358	0.00000000
H	-16.98452074	-9.80236459	0.00000000
H	-16.98456421	9.80235115	0.00000000
H	-16.24179473	-0.96787605	0.00000000
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H	-15.74405252	-11.93179096	0.00000000
H	-15.74410731	11.93177837	0.00000000
H	-15.06875255	-3.06307642	0.00000000
H	-15.06876853	3.06308244	0.00000000
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H	-12.65188349	-7.29472458	0.00000000
H	-12.65192223	7.29473059	0.00000000
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H	-11.96791793	18.24856383	0.00000000
H	-11.42593307	-9.40009470	0.00000000
H	-11.42598173	9.40010024	0.00000000
H	-10.18740180	-11.49963465	0.00000000
H	-10.18745840	11.49964111	0.00000000
H	-9.82204789	-19.48559197	0.00000000
H	-9.82212851	19.48560753	0.00000000
H	-8.95564023	-13.56246697	0.00000000
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H	-7.41515598	-19.51406622	0.00000000
H	-7.27698781	-14.53057671	0.00000000
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H	-4.93065462	-19.56687222	0.00000000
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H	-4.87468122	14.56235659	0.00000000
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H	2.43685324	-14.58191821	0.00000000
H	2.43686277	14.58193112	0.00000000
H	2.46362626	19.58755242	0.00000000
H	4.93063369	-19.56688816	0.00000000
H	4.87462758	-14.56235729	0.00000000
H	4.87465470	14.56236964	0.00000000
H	4.93066721	19.56691947	0.00000000
H	7.41513672	-19.51409064	0.00000000
H	7.27698443	-14.53059734	0.00000000
H	7.27702362	14.53060908	0.00000000
H	7.41518649	19.51411598	0.00000000
H	8.95563850	-13.56249121	0.00000000
H	8.95568431	13.56249709	0.00000000
H	9.82203206	-19.48562315	0.00000000
H	9.82209396	19.48563927	0.00000000
H	10.18740470	-11.49965868	0.00000000
H	10.18744709	11.49965803	0.00000000
H	11.42594137	-9.40011770	0.00000000
H	11.42597872	9.40011144	0.00000000

H	11.96782642	-18.24859464	0.00000000
H	11.96788944	18.24860087	0.00000000
H	12.65189718	-7.29474617	0.00000000
H	12.65192802	7.29473480	0.00000000
H	13.19887319	-16.18010055	0.00000000
H	13.19893297	16.18009637	0.00000000
H	13.86625882	-5.18288615	0.00000000
H	13.86628180	5.18287001	0.00000000
H	14.48961873	-14.05669337	0.00000000
H	14.48967263	14.05668010	0.00000000
H	15.06877715	-3.06309375	0.00000000
H	15.06879121	3.06307300	0.00000000
H	15.74406318	-11.93182666	0.00000000
H	15.74411054	11.93180540	0.00000000
H	16.24182476	-0.96789122	0.00000000
H	16.24182953	0.96786540	0.00000000
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H	18.21267532	-7.66556818	0.00000000
H	18.21270712	7.66553416	0.00000000
H	19.42978902	-5.51834437	0.00000000
H	19.42981228	5.51830498	0.00000000
H	20.62706472	-3.33898264	0.00000000
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H	21.80540065	-1.23832430	0.00000000
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10-HGQR (triplet)

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C	-23.31581908	0.68034154	0.00000000
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C	-22.10079024	1.42988370	0.00000000
C	-22.11552988	2.81697743	0.00000000
C	-20.92962948	-4.97966692	0.00000000
C	-20.93441148	-3.58202012	0.00000000
C	-20.84171917	-0.72517251	0.00000000
C	-20.84171896	0.72516377	0.00000000
C	-20.93441045	3.58201164	0.00000000
C	-20.92962810	4.97965860	0.00000000
C	-19.71962703	-7.12111801	0.00000000
C	-19.73919275	-5.71908244	0.00000000
C	-19.67333904	-2.87603784	0.00000000
C	-19.67636256	-1.46984223	0.00000000
C	-19.67636208	1.46983322	0.00000000
C	-19.67333811	2.87602895	0.00000000
C	-19.73919114	5.71907408	0.00000000
C	-19.71962513	7.12110992	0.00000000
C	-18.49927018	-9.25407549	0.00000000
C	-18.52694825	-7.85236477	0.00000000
C	-18.47490911	-5.00417107	0.00000000
C	-18.48509354	-3.60611506	0.00000000
C	-18.48509223	3.60610603	0.00000000
C	-18.47490744	5.00416235	0.00000000
C	-18.52694613	7.85235688	0.00000000
C	-18.49926786	9.25406800	0.00000000
C	-17.26827141	-11.38003149	0.00000000
C	-17.30238234	-9.98038115	0.00000000
C	-17.26440552	-7.12986141	0.00000000
C	-17.28173505	-5.73421409	0.00000000
C	-17.28173295	5.73420546	0.00000000
C	-17.26440317	7.12985325	0.00000000
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11-HGQR (triplet)

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12-HGQR (triplet)

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13-HGQR (triplet)

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14-HGQR (triplet)

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15-HGQR (triplet)

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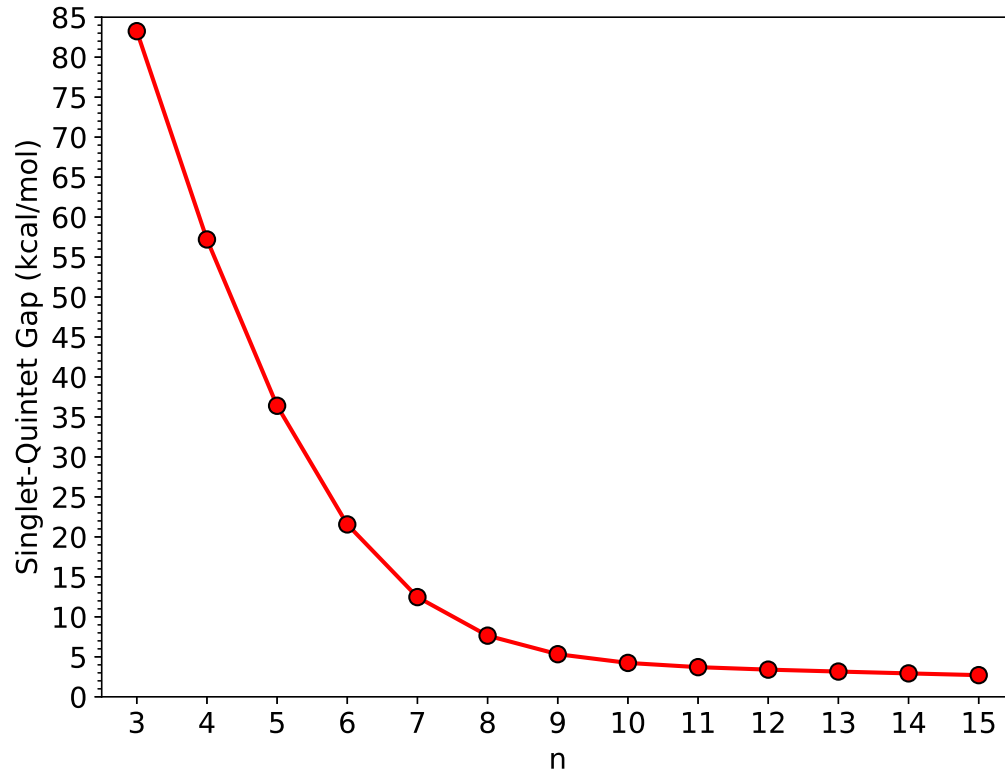
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H	-18.82527116	-22.09405634	0.00000000
H	-18.82527447	22.09405309	0.00000000
H	-17.56534740	-24.18883734	0.00000000
H	-17.56535006	24.18883411	0.00000000
H	-17.16716273	-32.18000182	0.00000000
H	-17.16716405	32.17999930	0.00000000
H	-16.31724557	-26.25127770	0.00000000
H	-16.31724787	26.25127437	0.00000000
H	-14.76696899	-32.20415275	0.00000000

H	-14.62845850	-27.22052175	0.00000000
H	-14.62845882	27.22051966	0.00000000
H	-14.76697057	32.20415041	0.00000000
H	-12.28934266	-32.26062809	0.00000000
H	-12.21804685	-27.25662260	0.00000000
H	-12.21804725	27.25662115	0.00000000
H	-12.28934434	32.26062630	0.00000000
H	-9.82816957	-32.29161377	0.00000000
H	-9.77340615	-27.28697421	0.00000000
H	-9.77340649	27.28697349	0.00000000
H	-9.82817124	32.29161254	0.00000000
H	-7.37044860	-32.31504005	0.00000000
H	-7.32966909	-27.31019008	0.00000000
H	-7.32966949	27.31019011	0.00000000
H	-7.37045035	32.31503938	0.00000000
H	-4.91350772	-32.33144462	0.00000000
H	-4.88642216	-27.32693398	0.00000000
H	-4.88642282	27.32693476	0.00000000
H	-4.91350970	32.33144452	0.00000000
H	-2.45675849	-32.34118041	0.00000000
H	-2.44324890	-27.33702989	0.00000000
H	-2.44325007	27.33703138	0.00000000
H	-2.45676090	32.34118088	0.00000000
H	0.00000972	-32.34440986	0.00000000
H	0.00000893	-27.34040066	0.00000000
H	0.00000696	27.34040276	0.00000000
H	0.00000673	32.34441086	0.00000000
H	2.45677786	-32.34117946	0.00000000
H	2.44326655	-27.33702922	0.00000000
H	2.44326369	27.33703178	0.00000000
H	2.45677411	32.34118097	0.00000000
H	4.91352665	-32.33144268	0.00000000
H	4.88643933	-27.32693264	0.00000000
H	4.88643551	27.32693551	0.00000000
H	4.91352217	32.33144463	0.00000000
H	7.37046677	-32.31503710	0.00000000
H	7.32968544	-27.31018808	0.00000000
H	7.32968077	27.31019110	0.00000000
H	7.37046169	32.31503941	0.00000000
H	9.82818664	-32.29160977	0.00000000
H	9.77342129	-27.28697154	0.00000000
H	9.77341599	27.28697456	0.00000000
H	9.82818119	32.29161233	0.00000000
H	12.28935838	-32.26062291	0.00000000
H	12.21806030	-27.25661924	0.00000000
H	12.21805469	27.25662213	0.00000000
H	12.28935279	32.26062559	0.00000000
H	14.76698292	-32.20414599	0.00000000
H	14.62846988	-27.22051755	0.00000000
H	14.62846417	27.22052026	0.00000000
H	14.76697734	32.20414872	0.00000000
H	16.31725423	-26.25127548	0.00000000
H	16.31724936	26.25127745	0.00000000
H	17.16717392	-32.17999397	0.00000000
H	17.16716850	32.17999683	0.00000000
H	17.56535425	-24.18883956	0.00000000
H	17.56534964	24.18884072	0.00000000
H	18.82527488	-22.09406439	0.00000000
H	18.82527085	22.09406434	0.00000000
H	19.31702884	-30.94656802	0.00000000
H	19.31702379	30.94657087	0.00000000
H	20.07785456	-19.99652536	0.00000000
H	20.07785128	19.99652383	0.00000000
H	20.54956628	-28.88679138	0.00000000
H	20.54956178	28.88679380	0.00000000
H	21.32358976	-17.89592926	0.00000000
H	21.32358732	17.89592619	0.00000000
H	21.84882817	-26.77656959	0.00000000
H	21.84882430	26.77657128	0.00000000
H	22.56229136	-15.79163312	0.00000000
H	22.56228970	15.79162867	0.00000000
H	23.11805634	-24.66717582	0.00000000
H	23.11805331	24.66717637	0.00000000
H	23.79376195	-13.68329608	0.00000000
H	23.79376093	13.68329058	0.00000000
H	24.37868438	-22.55626821	0.00000000
H	24.37868229	22.55626734	0.00000000
H	25.01777153	-11.57084203	0.00000000
H	25.01777096	11.57083589	0.00000000
H	25.63218994	-20.44167665	0.00000000
H	25.63218877	20.44167424	0.00000000
H	26.23416029	-9.45423452	0.00000000
H	26.23415996	9.45422814	0.00000000

H	26.87887260	-18.32295859	0.00000000
H	26.87887218	18.32295475	0.00000000
H	27.44298766	-7.33327834	0.00000000
H	27.44298743	7.33327200	0.00000000
H	28.11871879	-16.19992388	0.00000000
H	28.11871888	16.19991892	0.00000000
H	28.64458085	-5.20762522	0.00000000
H	28.64458066	5.20761905	0.00000000
H	29.35153669	-14.07254902	0.00000000
H	29.35153702	14.07254334	0.00000000
H	29.83863690	-3.07646757	0.00000000
H	29.83863678	3.07646159	0.00000000
H	30.57709166	-11.94079274	0.00000000
H	30.57709203	11.94078674	0.00000000
H	31.00837120	-0.97162065	0.00000000
H	31.00837115	0.97161486	0.00000000
H	31.79520625	-9.80438749	0.00000000
H	31.79520652	9.80438146	0.00000000
H	33.00577369	-7.66267790	0.00000000
H	33.00577383	7.66267199	0.00000000
H	34.20962727	-5.51316124	0.00000000
H	34.20962730	5.51315549	0.00000000
H	35.39782378	-3.33512556	0.00000000
H	35.39782378	3.33511990	0.00000000
H	36.57295811	-1.23900917	0.00000000
H	36.57295808	1.23900359	0.00000000

FIGURES

FIG. S1. Singlet-quintet gap of n -HGQR, calculated by spin-unrestricted TAO-LDA.

TABLES

TABLE S1. Singlet-triplet gap E_{ST} (in kcal/mol) of n -HGQR, calculated by spin-unrestricted KS-LDA and TAO-LDA.

n	KS-LDA	TAO-LDA
3	51.14	36.03
4	40.03	23.10
5	31.33	13.18
6	12.63	6.74
7	15.27	3.42
8	10.34	1.96
9	6.51	1.33
10	3.30	1.05
11	0.90	0.91
12	1.12	0.84
13	2.03	0.78
14	2.38	0.73
15		0.68

TABLE S2. Vertical ionization potential IP_v (in eV), vertical electron affinity EA_v (in eV), fundamental gap E_g (in eV), and symmetrized von Neumann entropy S_{vN} of ground-state n -HGQR, calculated by spin-unrestricted TAO-LDA.

n	IP_v	EA_v	E_g	S_{vN}
3	5.95	1.62	4.33	0.09
4	5.40	2.22	3.18	0.33
5	5.01	2.64	2.37	0.95
6	4.74	2.91	1.83	2.14
7	5.58	3.09	1.49	3.79
8	4.48	3.19	1.29	5.59
9	4.41	3.27	1.15	7.18
10	4.36	3.32	1.04	8.47
11	4.32	3.36	0.96	9.54
12	4.29	3.40	0.89	10.54
13	4.26	3.43	0.83	11.55
14	4.23	3.45	0.78	12.62
15	4.21	3.48	0.73	13.74