

Polycyclic Antiaromatic Hydrocarbons

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Molecular structures

Table 1: The Cartesian coordinates (in bohr) of **1** as obtained at the BP/SV(P) level.

-5.19044708243907	-1.29904249589042	0.00000000000000	c
-5.19044708243907	1.29904249589042	0.00000000000000	c
-2.94517899246921	2.76979121208140	0.00000000000000	c
-0.92612005660678	3.93549543221129	0.00000000000000	c
1.47021973918289	5.14458027833626	0.00000000000000	c
3.72022734325618	3.84553778244585	0.00000000000000	c
3.87129904907598	1.16570422012989	0.00000000000000	c
3.87129904907598	-1.16570422012989	0.00000000000000	c
3.72022734325618	-3.84553778244585	0.00000000000000	c
1.47021973918289	-5.14458027833626	0.00000000000000	c
-0.92612005660678	-3.93549543221129	0.00000000000000	c
-2.94517899246921	-2.76979121208140	0.00000000000000	c
-7.02636348752549	-2.29413725460972	0.00000000000000	h
-7.02636348752549	2.29413725460972	0.00000000000000	h
5.49996288602305	4.93794064911564	0.00000000000000	h
1.52640060150244	7.23207790372536	0.00000000000000	h
5.49996288602305	-4.93794064911564	0.00000000000000	h
1.52640060150244	-7.23207790372536	0.00000000000000	h

Table 2: The Cartesian coordinates (in bohr) of **2** as obtained at the BP/SV(P) level.

2.72066411120542	0.000000000000000	0.72059940072064	c
1.36093589958086	0.000000000000000	3.05215067955167	c
-2.72066411120542	0.000000000000000	0.72059940072064	c
3.85993299894181	0.000000000000000	-1.31347903290341	c
5.08850530169200	0.000000000000000	-3.68913462654568	c
1.16794547875006	0.000000000000000	-6.16624684791417	c
-1.16794547875006	0.000000000000000	-6.16624684791417	c
-3.82959176255280	0.000000000000000	-5.97079427159395	c
-5.08850530169200	0.000000000000000	-3.68913462654568	c
-3.85993299894181	0.000000000000000	-1.31347903290341	c
3.82959176255280	0.000000000000000	-5.97079427159395	c
7.17734404361671	0.000000000000000	-3.71211127614189	h
-4.96036854969919	0.000000000000000	-7.72678205140804	h
-7.17734404361671	0.000000000000000	-3.71211127614189	h
4.96036854969919	0.000000000000000	-7.72678205140804	h
-2.65253491396900	0.000000000000000	5.38847096630188	c
2.65253491396900	0.000000000000000	5.38847096630188	c
1.32554573588724	0.000000000000000	7.69092011862503	c
2.37828123262429	0.000000000000000	9.48818697740686	h
-2.37828123262429	0.000000000000000	9.48818697740686	h
-1.32554573588724	0.000000000000000	7.69092011862503	c
-1.36093589958086	0.000000000000000	3.05215067955167	c
-4.73360369592739	0.000000000000000	5.37676976660316	h
4.73360369592739	0.000000000000000	5.37676976660316	h

Table 3: The Cartesian coordinates (in bohr) of **3** as obtained at the BP/SV(P) level.

-4.65983612414185	2.72287482534033	0.00000000000000	c
-2.33810234673720	1.35934245760178	0.00000000000000	c
-4.65983612414185	-2.72287482534033	0.00000000000000	c
-6.69422940627598	3.86397804056242	0.00000000000000	c
-9.06841434263069	5.09189387208706	0.00000000000000	c
-11.54045742191924	1.16788139208346	0.00000000000000	c
-11.54045742191924	-1.16788139208346	0.00000000000000	c
-11.34883799783377	-3.82955180148283	0.00000000000000	c
-9.06841434263069	-5.09189387208706	0.00000000000000	c
-6.69422940627598	-3.86397804056242	0.00000000000000	c
-11.34883799783377	3.82955180148283	0.00000000000000	c
-9.09179749329279	7.18040192036553	0.00000000000000	h
-13.10647174909692	-4.95756479222356	0.00000000000000	h
-9.09179749329279	-7.18040192036553	0.00000000000000	h
-13.10647174909692	4.95756479222356	0.00000000000000	h
0.00000000000000	-2.64806268148488	0.00000000000000	c
0.00000000000000	2.64806268148488	0.00000000000000	c
2.33810234673720	1.35934245760178	0.00000000000000	c
4.65983612414185	2.72287482534033	0.00000000000000	c
6.69422940627597	3.86397804056242	0.00000000000000	c
9.06841434263068	5.09189387208707	0.00000000000000	c
11.34883799783377	3.82955180148283	0.00000000000000	c
11.54045742191923	1.16788139208346	0.00000000000000	c
11.54045742191923	-1.16788139208346	0.00000000000000	c
11.34883799783377	-3.82955180148283	0.00000000000000	c
9.06841434263068	-5.09189387208707	0.00000000000000	c
6.69422940627597	-3.86397804056242	0.00000000000000	c
4.65983612414185	-2.72287482534033	0.00000000000000	c
2.33810234673720	-1.35934245760178	0.00000000000000	c
-2.33810234673720	-1.35934245760178	0.00000000000000	c
0.00000000000000	-4.72700619804895	0.00000000000000	h
0.00000000000000	4.72700619804895	0.00000000000000	h
9.09179749329278	7.18040192036553	0.00000000000000	h
13.10647174909692	4.95756479222356	0.00000000000000	h
13.10647174909692	-4.95756479222356	0.00000000000000	h
9.09179749329278	-7.18040192036553	0.00000000000000	h

Table 4: The Cartesian coordinates (in bohr) of **4** as obtained at the BP/SV(P) level.

10.68060538715213	0.000000000000000	-9.48604554454647	h
15.26746493307019	0.000000000000000	-9.64085407072962	h
14.33913026979104	0.000000000000000	-7.77019443325418	c
15.86968029423325	0.000000000000000	-5.58592768948395	c
17.06974832886582	0.000000000000000	-3.58130306400801	c
18.26907033778161	0.000000000000000	-1.19914624066270	c
16.95758032548155	0.000000000000000	1.05398527066623	c
14.29042558754771	0.000000000000000	1.21741781434292	c
11.95882344713566	0.000000000000000	1.28527040267867	c
9.26664039119071	0.000000000000000	1.30888031078653	c
9.16175642174802	0.000000000000000	-3.38927675145006	c
10.32724668500039	0.000000000000000	-5.40984699258785	c
11.73324077892245	0.000000000000000	-7.68179911294640	c
20.35635331690010	0.000000000000000	-1.13072990457969	h
18.04837890670656	0.000000000000000	2.83516270382289	h
7.92566501124801	0.000000000000000	3.61001915102657	c
5.20439800367946	0.000000000000000	-0.93593925349533	c
5.25180047657007	0.000000000000000	3.70660047355637	c
3.85502450600156	0.000000000000000	1.37298413665570	c
3.96291615436013	0.000000000000000	6.05878279922691	c
2.76886864897515	0.000000000000000	8.06465737650219	c
1.30044045796914	0.000000000000000	10.28789550647686	c
-1.30044045796914	0.000000000000000	10.28789550647686	c
-2.76886864897515	0.000000000000000	8.06465737650219	c
-3.96291615436013	0.000000000000000	6.05878279922691	c
-3.85502450600156	0.000000000000000	1.37298413665570	c
-1.16475189147725	0.000000000000000	1.36694762268392	c
1.16475189147725	0.000000000000000	1.36694762268392	c
7.86739589853559	0.000000000000000	-1.02906711351649	c
2.29005561289473	0.000000000000000	12.12718278951939	h
-2.29005561289473	0.000000000000000	12.12718278951939	h
8.99037223694874	0.000000000000000	5.39520923471373	h
4.13839671979594	0.000000000000000	-2.72045724533834	h
-7.92566501124801	0.000000000000000	3.61001915102657	c
-5.20439800367946	0.000000000000000	-0.93593925349533	c
-9.26664039119071	0.000000000000000	1.30888031078653	c
-7.86739589853559	0.000000000000000	-1.02906711351649	c
-11.95882344713566	0.000000000000000	1.28527040267867	c

-14.29042558754771	0.000000000000000	1.21741781434292	c
-16.95758032548155	0.000000000000000	1.05398527066623	c
-18.26907033778161	0.000000000000000	-1.19914624066270	c
-17.06974832886582	0.000000000000000	-3.58130306400801	c
-15.86968029423325	0.000000000000000	-5.58592768948395	c
-14.33913026979104	0.000000000000000	-7.77019443325418	c
-11.73324077892245	0.000000000000000	-7.68179911294640	c
-10.32724668500039	0.000000000000000	-5.40984699258785	c
-9.16175642174802	0.000000000000000	-3.38927675145006	c
-5.25180047657007	0.000000000000000	3.70660047355637	c
-8.99037223694874	0.000000000000000	5.39520923471373	h
-4.13839671979594	0.000000000000000	-2.72045724533834	h
-18.04837890670656	0.000000000000000	2.83516270382289	h
-20.35635331690010	0.000000000000000	-1.13072990457969	h
-15.26746493307019	0.000000000000000	-9.64085407072962	h
-10.68060538715213	0.000000000000000	-9.48604554454647	h

Table 5: The Cartesian coordinates (in bohr) of **5** as obtained at the BP/SV(P) level.

0.0000000000000000	-11.94905695497427	8.15556317051807	c
0.0000000000000000	-9.26620274565038	8.18481450334599	c
0.0000000000000000	-9.14007622682516	3.47954714196107	c
0.0000000000000000	-14.28074941447340	8.04672130304173	c
0.0000000000000000	-16.93409543982770	7.80258757247995	c
0.0000000000000000	-16.89806431109653	3.15897346960343	c
0.0000000000000000	-15.69180125279767	1.16003749999064	c
0.0000000000000000	-14.22200554606860	-1.08266388702077	c
0.0000000000000000	-10.24265747408473	1.42558321990434	c
0.0000000000000000	-18.16618749365564	5.50161151978578	c
0.0000000000000000	-18.08649714274977	9.54423171477757	h
0.0000000000000000	-20.25461913339247	5.49528972076493	h
0.0000000000000000	-5.19840624877139	5.94295699093818	c
0.0000000000000000	-7.92285082827827	10.49085177544614	c
0.0000000000000000	-5.25466142943794	10.58708965866069	c
0.0000000000000000	-3.96512791018297	12.93900504530236	c
0.0000000000000000	-2.77073728860443	14.94485619322804	c
0.0000000000000000	-1.30512208453647	17.16923416602835	c
0.0000000000000000	1.30512208453647	17.16923416602835	c
0.0000000000000000	2.77073728860443	14.94485619322804	c
0.0000000000000000	3.96512791018297	12.93900504530236	c
0.0000000000000000	5.25466142943794	10.58708965866069	c
0.0000000000000000	1.16555794947349	8.25438687856186	c
0.0000000000000000	-1.16555794947349	8.25438687856186	c
0.0000000000000000	-3.85344394081366	8.24928064467410	c
0.0000000000000000	-7.86538116481490	5.84638671085420	c
0.0000000000000000	-4.13106359820571	4.15928062992730	h
0.0000000000000000	-8.99019042866459	12.27464655105168	h
0.0000000000000000	-2.29740357378836	19.00695451388146	h
0.0000000000000000	2.29740357378836	19.00695451388146	h
0.0000000000000000	7.92285082827827	10.49085177544614	c
0.0000000000000000	5.19840624877139	5.94295699093818	c
0.0000000000000000	9.26620274565038	8.18481450334599	c
0.0000000000000000	7.86538116481490	5.84638671085420	c
0.0000000000000000	11.94905695497427	8.15556317051807	c
0.0000000000000000	14.28074941447340	8.04672130304173	c
0.0000000000000000	16.93409543982770	7.80258757247995	c
0.0000000000000000	18.16618749365564	5.50161151978578	c

0.0000000000000000	16.89806431109653	3.15897346960343	c
0.0000000000000000	15.69180125279767	1.16003749999064	c
0.0000000000000000	11.50563429690753	-0.94706708741289	c
0.0000000000000000	10.24265747408473	1.42558321990434	c
0.0000000000000000	9.14007622682516	3.47954714196107	c
0.0000000000000000	3.85344394081366	8.24928064467410	c
0.0000000000000000	18.08649714274977	9.54423171477757	h
0.0000000000000000	20.25461913339247	5.49528972076493	h
0.0000000000000000	8.99019042866459	12.27464655105168	h
0.0000000000000000	4.13106359820571	4.15928062992730	h
0.0000000000000000	15.39372182731925	-3.48901820486247	c
0.0000000000000000	10.10124281805269	-3.22350186652623	c
0.0000000000000000	13.99241864281883	-5.75338324571542	c
0.0000000000000000	11.27017246603379	-5.61750881328397	c
0.0000000000000000	-10.10124281805269	-3.22350186652623	c
0.0000000000000000	-15.39372182731925	-3.48901820486247	c
0.0000000000000000	-11.27017246603379	-5.61750881328397	c
0.0000000000000000	-13.99241864281883	-5.75338324571542	c
0.0000000000000000	15.23561149880770	-8.14170190153655	c
0.0000000000000000	16.26799858925739	-10.23351201644111	c
0.0000000000000000	17.37711239322667	-12.66454660643951	c
0.0000000000000000	16.00380182816132	-14.88083193305418	c
0.0000000000000000	13.33742134068978	-14.94085338698560	c
0.0000000000000000	11.00409508007673	-14.82437214874848	c
0.0000000000000000	8.35716682776009	-14.49752766553339	c
0.0000000000000000	7.21253177533738	-12.15461026463171	c
0.0000000000000000	8.55752020391507	-9.84636373511640	c
0.0000000000000000	9.79501048272718	-7.86886003429403	c
0.0000000000000000	-9.79501048272718	-7.86886003429403	c
0.0000000000000000	-8.55752020391507	-9.84636373511640	c
0.0000000000000000	-7.21253177533738	-12.15461026463171	c
0.0000000000000000	-8.35716682776009	-14.49752766553339	c
0.0000000000000000	-11.00409508007673	-14.82437214874848	c
0.0000000000000000	-13.33742134068978	-14.94085338698560	c
0.0000000000000000	-16.00380182816132	-14.88083193305418	c
0.0000000000000000	-17.37711239322667	-12.66454660643951	c
0.0000000000000000	-16.26799858925739	-10.23351201644111	c
0.0000000000000000	-15.23561149880770	-8.14170190153655	c
0.0000000000000000	14.22200554606860	-1.08266388702077	c

0.0000000000000000	-11.50563429690753	-0.94706708741289	c
0.0000000000000000	17.47009418959185	-3.59143515620676	h
0.0000000000000000	8.02502450521444	-3.11952396032137	h
0.0000000000000000	-8.02502450521444	-3.11952396032137	h
0.0000000000000000	-17.47009418959185	-3.59143515620676	h
0.0000000000000000	19.46192545654867	-12.79068978304444	h
0.0000000000000000	17.04424418881683	-16.69177874036530	h
0.0000000000000000	7.14074331376990	-16.19509414083609	h
0.0000000000000000	5.12552463364855	-12.07152041299475	h
0.0000000000000000	-5.12552463364855	-12.07152041299475	h
0.0000000000000000	-7.14074331376990	-16.19509414083609	h
0.0000000000000000	-17.04424418881683	-16.69177874036530	h
0.0000000000000000	-19.46192545654867	-12.79068978304444	h

Table 6: The Cartesian coordinates (in bohr) of **6** as obtained at the BP/SV(P) level.

16.05961136926673	-3.91632949452169	0.00000000000000	c
13.71672163087058	-5.22063051931229	0.00000000000000	c
11.33184884937559	-1.16597646448472	0.00000000000000	c
18.08545703442164	-2.75685259469959	0.00000000000000	c
20.31849906329913	-1.30482886654317	0.00000000000000	c
18.08545703442164	2.75685259469959	0.00000000000000	c
16.05961136926673	3.91632949452169	0.00000000000000	c
13.71672163087058	5.22063051931229	0.00000000000000	c
11.33184884937559	1.16597646448472	0.00000000000000	c
20.31849906329913	1.30482886654317	0.00000000000000	c
22.15328616742653	-2.30225947093994	0.00000000000000	h
22.15328616742653	2.30225947093994	0.00000000000000	h
9.07261591938260	-5.23807724330963	0.00000000000000	c
13.66235876325086	-7.88796650972813	0.00000000000000	c
11.37955946893208	-9.26871412931729	0.00000000000000	c
11.42144651647942	-11.94986667342953	0.00000000000000	c
11.43023289870971	-14.28403893351132	0.00000000000000	c
11.28926447766721	-16.94392192231578	0.00000000000000	c
9.02923458563191	-18.24875078885896	0.00000000000000	c
6.65522413571192	-17.04089152821092	0.00000000000000	c
4.63816485278730	-15.86619616795122	0.00000000000000	c
2.33716216193849	-14.48934464862959	0.00000000000000	c
4.65615918622926	-10.39665720764708	0.00000000000000	c
6.67568966314633	-9.23068074316236	0.00000000000000	c
9.01728712237253	-7.90813813452522	0.00000000000000	c
11.35729208232159	-3.85513065393027	0.00000000000000	c
7.27196377943091	-4.19847024559164	0.00000000000000	h
15.46288760816017	-8.92750232302020	0.00000000000000	h
13.07045827165058	-18.03417886282780	0.00000000000000	h
9.08282789577594	-20.33643833376776	0.00000000000000	h
0.00000000000000	-15.77593301945626	0.00000000000000	c
0.00000000000000	-10.47615448661925	0.00000000000000	c
-2.33716216193850	-14.48934464862959	0.00000000000000	c
-2.34000495994907	-11.76326878845549	0.00000000000000	c
-4.63816485278731	-15.86619616795122	0.00000000000000	c
-6.65522413571193	-17.04089152821091	0.00000000000000	c
-9.02923458563191	-18.24875078885895	0.00000000000000	c
-11.28926447766721	-16.94392192231577	0.00000000000000	c

-11.43023289870971	-14.28403893351132	0.00000000000000	c
-11.42144651647942	-11.94986667342953	0.00000000000000	c
-9.01728712237252	-7.90813813452523	0.00000000000000	c
-6.67568966314633	-9.23068074316235	0.00000000000000	c
-4.65615918622926	-10.39665720764708	0.00000000000000	c
2.34000495994907	-11.76326878845549	0.00000000000000	c
-9.08282789577594	-20.33643833376775	0.00000000000000	h
-13.07045827165058	-18.03417886282780	0.00000000000000	h
0.00000000000000	-17.85500464604040	0.00000000000000	h
0.00000000000000	-8.39694049118329	0.00000000000000	h
-13.66235876325086	-7.88796650972813	0.00000000000000	c
-9.07261591938260	-5.23807724330963	0.00000000000000	c
-13.71672163087058	-5.22063051931229	0.00000000000000	c
-11.35729208232159	-3.85513065393027	0.00000000000000	c
9.07261591938260	5.23807724330963	0.00000000000000	c
13.66235876325086	7.88796650972813	0.00000000000000	c
9.01728712237253	7.90813813452522	0.00000000000000	c
11.37955946893208	9.26871412931729	0.00000000000000	c
-16.05961136926673	-3.91632949452169	0.00000000000000	c
-18.08545703442164	-2.75685259469960	0.00000000000000	c
-20.31849906329913	-1.30482886654318	0.00000000000000	c
-20.31849906329913	1.30482886654318	0.00000000000000	c
-18.08545703442164	2.75685259469960	0.00000000000000	c
-16.05961136926673	3.91632949452169	0.00000000000000	c
-13.71672163087058	5.22063051931229	0.00000000000000	c
-11.33184884937558	1.16597646448472	0.00000000000000	c
-11.33184884937558	-1.16597646448472	0.00000000000000	c
6.67568966314633	9.23068074316236	0.00000000000000	c
4.65615918622926	10.39665720764708	0.00000000000000	c
2.33716216193849	14.48934464862959	0.00000000000000	c
4.63816485278730	15.86619616795122	0.00000000000000	c
6.65522413571192	17.04089152821092	0.00000000000000	c
9.02923458563191	18.24875078885896	0.00000000000000	c
11.28926447766721	16.94392192231578	0.00000000000000	c
11.43023289870971	14.28403893351132	0.00000000000000	c
11.42144651647942	11.94986667342953	0.00000000000000	c
-11.37955946893208	-9.26871412931729	0.00000000000000	c
11.35729208232159	3.85513065393027	0.00000000000000	c
-15.46288760816016	-8.92750232302020	0.00000000000000	h

-7.27196377943091	-4.19847024559164	0.00000000000000	h
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-22.15328616742653	-2.30225947093995	0.00000000000000	h
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9.08282789577594	20.33643833376776	0.00000000000000	h
13.07045827165058	18.03417886282780	0.00000000000000	h
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