

ELECTRONIC SUPPLEMENTARY INFORMATION

Relations between the aromaticity and magnetic dipole transitions in the electronic spectra of hetero[8]circulenes

R. R. Valiev^{a,b,*}, G. V. Baryshnkiov^{a,c}, D. Sundholm^b

^a*Tomsk State University, 36 Lenin Avenue, 634050, Tomsk, Russian Federation,*

E-mail: valievrashid@gmail.com

^b*Department of Chemistry, University of Helsinki, P.O. Box 55 (A.I. Virtanens plats 1), Helsinki FIN-00014, Finland*

^c*Division of Theoretical Chemistry and Biology, School of Engineering Sciences in Chemistry, Biotechnology and Health, KTH Royal Institute of Technology, 10691 Stockholm, Sweden*

Contents

1. The energy and order of orbitals for II^{2+} and IV^{2+}	1
2. The Cartesian coordinates of atoms in Å for the neutral molecules.....	2
3. The Cartesian coordinates of atoms in Å for the dications.....	11
4. The Cartesian coordinates of atoms in Å for the dianions	21

1. The energy and order of MOs for II^{2+} and IV^{2+}

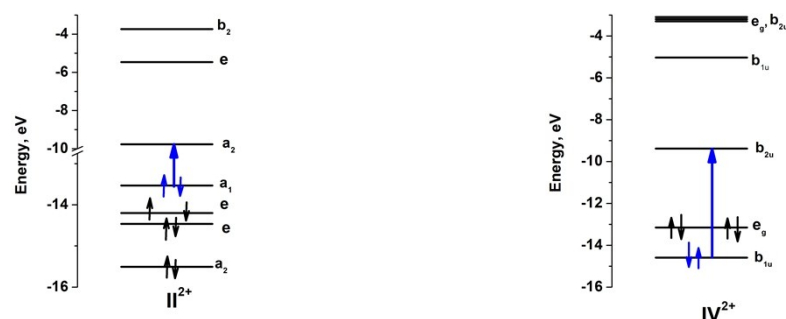


Figure S1. The energies and order of MOs for II^{2+} and IV^{2+} .

2. The Cartesian coordinates of atoms in Å for the neutral molecules

2.1. I

C	0.701211000	4.166577000	0.000000000
C	-0.701211000	4.166577000	0.000000000
C	-1.371918000	2.937335000	0.000000000
C	-0.697967000	1.710319000	0.000000000
C	0.697967000	1.710319000	0.000000000
C	1.371918000	2.937335000	0.000000000
O	2.743638000	2.743638000	0.000000000
C	2.937335000	1.371918000	0.000000000
C	1.710319000	0.697967000	0.000000000
C	4.166577000	0.701211000	0.000000000
C	4.166577000	-0.701211000	0.000000000
H	1.252091000	5.100140000	0.000000000
H	-1.252091000	5.100140000	0.000000000
H	5.100140000	1.252091000	0.000000000
H	5.100140000	-1.252091000	0.000000000
C	1.710319000	-0.697967000	0.000000000
C	2.937335000	-1.371918000	0.000000000
O	2.743638000	-2.743638000	0.000000000
C	1.371918000	-2.937335000	0.000000000
C	0.697967000	-1.710319000	0.000000000
C	0.701211000	-4.166577000	0.000000000
C	-0.701211000	-4.166577000	0.000000000
H	1.252091000	-5.100140000	0.000000000
H	-1.252091000	-5.100140000	0.000000000
C	-0.697967000	-1.710319000	0.000000000
C	-1.371918000	-2.937335000	0.000000000

O	-2.743638000	-2.743638000	0.000000000
C	-2.937335000	-1.371918000	0.000000000
C	-1.710319000	-0.697967000	0.000000000
C	-4.166577000	-0.701211000	0.000000000
C	-4.166577000	0.701211000	0.000000000
C	-2.937335000	1.371918000	0.000000000
C	-1.710319000	0.697967000	0.000000000
H	-5.100140000	-1.252091000	0.000000000
H	-5.100140000	1.252091000	0.000000000
O	-2.743638000	2.743638000	0.000000000

2.2. II

C	-1.225131000	3.109466000	0.000050000
C	-3.109466000	1.225131000	-0.000050000
S	-4.334247000	0.000000000	-0.000097000
H	4.582526000	2.804038000	-0.000054000
H	2.804038000	4.582526000	0.000054000
C	3.109466000	1.225131000	-0.000050000
S	4.334247000	0.000000000	-0.000097000
C	3.109466000	-1.225131000	-0.000050000
C	1.765323000	-0.741739000	-0.000019000
C	1.765323000	0.741739000	-0.000019000
C	3.525579000	2.559393000	-0.000030000
C	2.559393000	3.525579000	0.000030000
C	1.225131000	3.109466000	0.000050000
C	0.741739000	1.765323000	0.000019000
C	3.525579000	-2.559393000	-0.000030000
C	2.559393000	-3.525579000	0.000030000
C	1.225131000	-3.109466000	0.000050000
C	0.741739000	-1.765323000	0.000019000

H	2.804038000	-4.582526000	0.000054000
H	4.582526000	-2.804038000	-0.000054000
C	-0.741739000	1.765323000	0.000019000
C	-1.765323000	0.741739000	-0.000019000
C	-1.765323000	-0.741739000	-0.000019000
C	-0.741739000	-1.765323000	0.000019000
C	-1.225131000	-3.109466000	0.000050000
C	-2.559393000	-3.525579000	0.000030000
C	-3.525579000	-2.559393000	-0.000030000
C	-3.109466000	-1.225131000	-0.000050000
H	-4.582526000	-2.804038000	-0.000054000
H	-2.804038000	-4.582526000	0.000054000
S	0.000000000	-4.334247000	0.000097000
S	0.000000000	4.334247000	0.000097000
C	-2.559393000	3.525579000	0.000030000
C	-3.525579000	2.559393000	-0.000030000
H	-2.804038000	4.582526000	0.000054000
H	-4.582526000	2.804038000	-0.000054000

2.3. III

C	-1.254501000	3.012228000	0.533353000
P	0.000000000	4.130336000	1.211547000
C	-0.749542000	1.718086000	0.206314000
C	0.749542000	1.718086000	0.206314000
C	1.254501000	3.012228000	0.533353000
C	-1.718086000	0.749542000	-0.206314000
C	-1.718086000	-0.749542000	-0.206314000
C	-0.749542000	-1.718086000	0.206314000
C	0.749542000	-1.718086000	0.206314000
C	1.718086000	-0.749542000	-0.206314000

C	1.718086000	0.749542000	-0.206314000
C	3.012228000	1.254501000	-0.533353000
C	3.012228000	-1.254501000	-0.533353000
P	4.130336000	0.000000000	-1.211547000
C	3.429274000	2.563969000	-0.321227000
C	2.563969000	3.429274000	0.321227000
H	2.875577000	4.431215000	0.602060000
H	4.431215000	2.875577000	-0.602060000
C	3.429274000	-2.563969000	-0.321227000
C	2.563969000	-3.429274000	0.321227000
C	1.254501000	-3.012228000	0.533353000
P	0.000000000	-4.130336000	1.211547000
C	-1.254501000	-3.012228000	0.533353000
C	-2.563969000	-3.429274000	0.321227000
C	-3.429274000	-2.563969000	-0.321227000
C	-3.012228000	-1.254501000	-0.533353000
P	-4.130336000	0.000000000	-1.211547000
C	-3.012228000	1.254501000	-0.533353000
C	-3.429274000	2.563969000	-0.321227000
C	-2.563969000	3.429274000	0.321227000
H	-4.431215000	2.875577000	-0.602060000
H	-2.875577000	4.431215000	0.602060000
H	-4.431215000	-2.875577000	-0.602060000
H	-2.875577000	-4.431215000	0.602060000
H	2.875577000	-4.431215000	0.602060000
H	4.431215000	-2.875577000	-0.602060000
H	0.000000000	5.122267000	0.186402000
H	0.000000000	-5.122267000	0.186402000
H	-5.122267000	0.000000000	-0.186402000

H	5.122267000	0.000000000	-0.186402000
---	-------------	-------------	--------------

2.4. IV

C	-1.373943000	2.974664000	-0.000039000
C	-0.705943000	1.723476000	0.000000000
C	0.705944000	1.723476000	0.000000000
C	1.723476000	0.705943000	0.000000000
C	2.974664000	1.373943000	0.000039000
C	1.373944000	2.974664000	0.000036000
C	1.723476000	-0.705944000	-0.000001000
N	2.740687000	2.740687000	0.000162000
C	2.974664000	-1.373944000	-0.000036000
C	0.694729000	4.205353000	0.000027000
C	-0.694729000	4.205353000	-0.000032000
C	4.205353000	-0.694729000	-0.000027000
C	4.205353000	0.694729000	0.000032000
H	1.243297000	5.142561000	0.000052000
H	-1.243297000	5.142561000	-0.000058000
H	5.142561000	-1.243297000	-0.000052000
H	5.142561000	1.243297000	0.000058000
H	3.451973000	3.451972000	-0.000353000
C	-1.723476000	0.705944000	-0.000001000
C	-2.974664000	1.373944000	-0.000036000
C	-1.723476000	-0.705943000	0.000000000
C	-0.705944000	-1.723476000	0.000000000
C	0.705943000	-1.723476000	0.000000000
C	-2.974664000	-1.373943000	0.000039000
C	-1.373944000	-2.974664000	0.000036000
C	1.373943000	-2.974664000	-0.000039000
C	-4.205353000	-0.694729000	0.000032000

C	-4.205353000	0.694729000	-0.000027000
C	0.694729000	-4.205353000	-0.000032000
C	-0.694729000	-4.205353000	0.000027000
H	-5.142561000	-1.243297000	0.000058000
H	-5.142561000	1.243297000	-0.000052000
H	1.243297000	-5.142561000	-0.000058000
H	-1.243297000	-5.142561000	0.000052000
N	-2.740687000	-2.740687000	0.000162000
H	-3.451973000	-3.451972000	-0.000353000
N	-2.740687000	2.740687000	-0.000163000
N	2.740687000	-2.740687000	-0.000163000
H	-3.451972000	3.451973000	0.000354000
H	3.451972000	-3.451973000	0.000354000

2.5. V

C	-2.573508000	3.373082000	0.399693000
C	-3.373082000	2.573508000	-0.399693000
C	-2.940361000	1.285445000	-0.674802000
C	-1.688590000	0.749401000	-0.265498000
C	-0.749401000	1.688590000	0.265498000
C	-1.285445000	2.940361000	0.674802000
As	-4.083803000	0.000000000	-1.571570000
C	-2.940361000	-1.285445000	-0.674802000
C	-1.688590000	-0.749401000	-0.265498000
C	-3.373082000	-2.573508000	-0.399693000
C	-2.573508000	-3.373082000	0.399693000
C	-1.285445000	-2.940361000	0.674802000
C	-0.749401000	-1.688590000	0.265498000
H	-2.920433000	-4.340483000	0.745641000
H	-4.340483000	-2.920433000	-0.745641000

H	-4.340483000	2.920433000	-0.745641000
H	-2.920433000	4.340483000	0.745641000
As	0.000000000	4.083803000	1.571570000
C	1.285445000	2.940361000	0.674802000
C	0.749401000	1.688590000	0.265498000
C	1.688590000	0.749401000	-0.265498000
C	2.940361000	1.285445000	-0.674802000
C	3.373082000	2.573508000	-0.399693000
C	2.573508000	3.373082000	0.399693000
C	1.688590000	-0.749401000	-0.265498000
C	2.940361000	-1.285445000	-0.674802000
As	4.083803000	0.000000000	-1.571570000
C	0.749401000	-1.688590000	0.265498000
C	1.285445000	-2.940361000	0.674802000
C	2.573508000	-3.373082000	0.399693000
C	3.373082000	-2.573508000	-0.399693000
H	2.920433000	-4.340483000	0.745641000
As	0.000000000	-4.083803000	1.571570000
H	4.340483000	-2.920433000	-0.745641000
H	4.340483000	2.920433000	-0.745641000
H	2.920433000	4.340483000	0.745641000
H	-5.193681000	0.000000000	-0.519322000
H	0.000000000	5.193681000	0.519322000
H	0.000000000	-5.193681000	0.519322000
H	5.193681000	0.000000000	-0.519322000

2.6. VI

C	1.357187665	3.008559235	0.000887150
C	2.842053866	2.842054567	0.000086454
C	0.703948661	1.752899505	0.001077446

C	1.752897453	0.703948756	0.000618700
C	3.008556931	1.357187803	-0.000227632
C	-0.703949133	1.752899541	0.000881560
C	-1.752898466	0.703949220	0.000174252
C	-1.752898440	-0.703949002	-0.000014233
C	-0.703948496	-1.752899625	0.000304134
C	0.703948959	-1.752899816	0.000389130
C	1.752897850	-0.703949284	0.000338757
C	3.008556894	-1.357188244	-0.000416106
C	1.357187883	-3.008559427	0.000544228
C	2.842053716	-2.842054952	-0.000111300
C	4.220978288	-0.693127574	-0.001275083
C	4.220978516	0.693127517	-0.001223953
H	5.148723060	1.253246886	-0.001784325
H	5.148722677	-1.253246941	-0.001812523
C	0.693128851	-4.220982279	0.000961190
C	-0.693126206	-4.220982706	0.001021806
C	-1.357186834	-3.008559770	0.000603953
C	-2.842053490	-2.842055389	0.000044606
C	-3.008557848	-1.357187866	-0.000453865
C	-4.220979997	-0.693126888	-0.001151749
C	-4.220980025	0.693128421	-0.001273284
C	-3.008558006	1.357189016	-0.000463663
C	-2.842053953	2.842055989	-0.000104055
C	-1.357187659	3.008559434	0.000727055
C	-0.693127161	4.220981629	0.000934847
C	0.693127643	4.220981707	0.000978761
H	-1.253247160	5.148725758	0.000945874
H	1.253247350	5.148725988	0.000937299

H	-5.148724256	1.253248135	-0.001880149
H	-5.148725071	-1.253245763	-0.001404118
H	-1.253245378	-5.148727480	0.001201567
H	1.253249185	-5.148726376	0.001119524
H	3.304768365	3.304136558	0.878608704
H	-3.304606227	-3.304007569	0.878721002
H	-3.304780320	3.304110792	0.878426340
H	3.304677976	-3.304129334	0.878462464
H	3.303790786	3.304423347	-0.878796117
H	3.303880799	-3.304431280	-0.878942380
H	-3.303951562	-3.304555438	-0.878683771
H	-3.303777685	3.304453201	-0.878978499

2.7. VII

C	-0.337209304	-3.203510035	0.659283644
C	-0.102215430	-1.810167091	0.277467952
C	-1.308142071	-1.211770028	-0.373334143
C	-1.787887420	0.099779455	-0.286035604
C	-3.146268618	0.333020909	-0.703635391
C	1.185714923	-1.308822938	0.397041815
C	1.787887362	-0.099779428	-0.286035604
C	1.308142034	1.211770049	-0.373334161
C	0.102215409	1.810167120	0.277467919
C	-1.185714949	1.308822993	0.397041766
C	-2.184460517	2.175715874	1.007395996
Si	-3.708273366	1.759841765	0.235173576
C	-1.823052986	3.363023639	1.690235763
C	-0.575044867	3.875834141	1.504688216
C	0.337209363	3.203510011	0.659283714
Si	1.558969799	3.908406040	-0.474205308

C	2.185261872	2.220668936	-0.904356654
C	3.146268538	-0.333020915	-0.703635425
C	3.905252982	0.626816869	-1.370124622
C	3.402145168	1.906265767	-1.500644570
H	4.005689554	2.684548915	-1.953327280
H	4.909875796	0.393598348	-1.704892792
H	2.593213807	4.849642390	0.038676374
H	-0.315485541	4.848551879	1.906789613
H	-2.568847364	3.905476084	2.260148940
H	-5.052715448	2.353246890	0.335789328
C	-3.905253070	-0.626816942	-1.370124486
C	-3.402145206	-1.906265826	-1.500644485
C	-2.185261844	-2.220668962	-0.904356676
Si	-1.558969579	-3.908406052	-0.474205545
C	0.575044896	-3.875834138	1.504688205
C	1.823052961	-3.363023546	1.690235852
C	2.184460487	-2.175715780	1.007396087
Si	3.708273322	-1.759841694	0.235173633
H	5.052715420	-2.353246776	0.335789426
H	2.568847316	-3.905475922	2.260149125
H	0.315485603	-4.848551902	1.906789560
H	-2.593213494	-4.849642610	0.038675941
H	-4.005689600	-2.684549001	-1.953327157
H	-4.909875938	-0.393598486	-1.704892541

3. Cartesian coordinates of atoms in Å for the dications

3.1. I

C	-3.364466740	2.514081376	0.000118011
C	-2.326320172	3.496972231	-0.000361096
C	-1.019620547	3.059137263	-0.000246403

C	-0.658934641	1.708653157	0.000397902
C	-1.669853833	0.751493835	0.000956047
C	-2.998614008	1.185551459	0.000877014
O	-3.852108101	0.063393846	0.000718341
C	-3.066319386	-1.015010975	0.000712562
C	-1.700744295	-0.658962043	0.000821464
C	-3.512264320	-2.383199421	0.000057849
C	-2.572021106	-3.376483506	-0.000457080
H	-4.401652468	2.821199195	-0.000487377
H	-2.576028958	4.549521609	-0.000958187
H	-4.570685448	-2.607200926	-0.000167225
H	-2.853488583	-4.421042234	-0.000806545
C	-0.751091893	-1.662150444	0.000093928
C	-1.181447758	-3.006174251	-0.000465510
O	-0.147378931	-3.849887834	-0.000936849
C	1.019486549	-3.059101544	-0.000674716
C	0.658931862	-1.708588981	-0.000076220
C	2.326114627	-3.497082989	-0.000525848
C	3.364387686	-2.514320669	0.000084038
H	2.575709872	-4.549655543	-0.000482919
H	4.401579344	-2.821574233	0.000323010
C	1.669922521	-0.751494408	0.000341456
C	2.998681919	-1.185683279	0.000422472
O	3.852312808	-0.063603587	0.000549016
C	3.066480024	1.015021412	0.000484254
C	1.700816465	0.658944750	0.000477691
C	3.512409151	2.383289295	0.000097351
C	2.572053613	3.376662447	-0.000579318
C	1.181422120	3.006341008	-0.000483696

C	0.751074017	1.662222280	0.000199017
H	4.570946734	2.607336410	0.000162569
H	2.853554438	4.421325041	-0.000957727
O	0.147157436	3.850070254	-0.000653276

3.2. II

C	-1.241943481	3.068133502	0.036906566
C	-3.094779959	1.173589401	-0.036345352
S	-4.294804338	-0.084436375	-0.068646378
H	4.551790385	2.869424380	-0.043198240
H	2.767995225	4.614218478	0.041729543
C	3.088938911	1.253125640	-0.035821524
S	4.295147436	0.084256137	-0.068574776
C	3.094871837	-1.173691916	-0.036329214
C	1.747672175	-0.704638456	-0.013720520
C	1.733116018	0.753620613	-0.012964670
C	3.499263184	2.618382932	-0.023052438
C	2.540272846	3.556386214	0.021991260
C	1.184401638	3.115945056	0.035447874
C	0.715040240	1.749422045	0.012979918
C	3.528585778	-2.481669462	-0.021752130
C	2.559002241	-3.472836755	0.022805908
C	1.241838917	-3.068044237	0.036836192
C	0.743148654	-1.731584319	0.013735503
H	2.828396645	-4.520773334	0.041267273
H	4.582246912	-2.727926137	-0.040030472
C	-0.743176503	1.731607419	0.013976117
C	-1.747646719	0.704610048	-0.013604044
C	-1.733135563	-0.753739979	-0.013096200
C	-0.715154786	-1.749448733	0.012810086

C	-1.184435723	-3.115861162	0.035393949
C	-2.540260331	-3.556265788	0.021928659
C	-3.499148605	-2.618366046	-0.022955098
C	-3.088855271	-1.253158969	-0.035915698
H	-4.551555858	-2.869360230	-0.042607474
H	-2.767940525	-4.613972550	0.041394338
S	0.010665257	-4.295644487	0.068722609
S	-0.010852985	4.295981806	0.068734121
C	-2.559161870	3.472790521	0.022746092
C	-3.528625133	2.481507812	-0.021834869
H	-2.828646639	4.520740962	0.041183237
H	-4.582270008	2.727675970	-0.040140149

3.3. III

C	-1.249035795	2.907973965	0.751517471
P	0.000345199	3.924562231	1.620986693
C	-0.707349767	1.656989280	0.290293781
C	0.707536114	1.657090781	0.289920593
C	1.249294303	2.908240148	0.750580682
C	-1.656956036	0.707436895	-0.289002750
C	-1.656896283	-0.707335204	-0.289541782
C	-0.707346426	-1.657157186	0.289448290
C	0.707316763	-1.657090854	0.289987508
C	1.657089041	-0.707420031	-0.288922370
C	1.657087536	0.707316360	-0.289101705
C	2.907986750	1.249019591	-0.750901095
C	2.907943113	-1.249301123	-0.750351971
P	3.923914606	-0.000335875	-1.621069093
C	3.311946997	2.522547555	-0.431477736
C	2.522387837	3.312472846	0.429639747

H	2.906695075	4.264467184	0.776242514
H	4.263447656	2.907004684	-0.779276477
C	3.311926860	-2.522546448	-0.430067563
C	2.522227714	-3.312170675	0.431242304
C	1.248997376	-2.908110810	0.751368557
P	-0.000375884	-3.924265535	1.621289380
C	-1.249276024	-2.908189830	0.750613295
C	-2.522358487	-3.312215733	0.429837421
C	-3.311689720	-2.522413315	-0.431663685
C	-2.907674101	-1.249019593	-0.751338483
P	-3.923761210	0.000404061	-1.621285902
C	-2.908017690	1.249257741	-0.750196234
C	-3.312218920	2.522464582	-0.429664136
C	-2.522490647	3.312002491	0.431625542
H	-4.263955950	2.906895541	-0.776885013
H	-2.906836420	4.263695182	0.779070443
H	-4.263017365	-2.907011678	-0.779686141
H	-2.906991835	-4.263907887	0.776821951
H	2.906660752	-4.263819716	0.778527967
H	4.263503939	-2.907098545	-0.777426702
H	-0.000144679	5.054153091	0.755209162
H	-0.000050106	-5.054250207	0.756079446
H	-5.053959198	-0.000192908	-0.756337595
H	5.054094913	-0.000141055	-0.756106316

3.4. IV

C	0.682287804	1.721794136	-0.001883098
C	1.363532976	2.975270561	-0.000506130
C	2.975392886	1.363602052	-0.000617633
C	1.721623535	0.682323929	-0.001990294

C	1.721674536	-0.682032338	-0.002107971
C	0.682117979	-1.721316889	-0.002188374
C	1.363507123	-2.975401351	-0.000667188
C	2.975149150	-1.363344198	-0.000769960
C	-0.682013874	-1.721334775	-0.002212469
C	-0.682180897	1.721813031	-0.001908691
C	-1.721449285	0.682263892	-0.002051944
C	-1.721497924	-0.681973347	-0.002185083
N	2.708651914	-2.709021279	-0.000057851
N	2.709189667	2.709002552	0.000060226
C	-1.363439815	2.975186407	-0.000537144
C	-2.975440016	1.363591255	-0.000657067
C	-1.363413456	-2.975316534	-0.000746944
N	-2.708660862	-2.708830680	-0.000150096
C	-2.975198973	-1.363335043	-0.000826307
C	4.205144821	-0.691465483	0.000388720
C	4.205194507	0.691373020	0.000479008
C	-0.691421541	-4.205316499	0.000690017
C	0.691392521	-4.205330603	0.000780341
C	-0.691442872	4.205083058	0.000671530
C	0.691412357	4.205098674	0.000677615
C	-4.205232068	-0.691458086	0.000431225
C	-4.205279618	0.691366616	0.000501043
H	5.138155025	-1.238964803	0.001280617
H	5.138297211	1.238694758	0.001452923
H	-1.238909203	-5.138352573	0.001893793
H	1.238817713	-5.138396689	0.002133562
H	-1.238823610	5.138150509	0.001618026
H	1.238729947	5.138198380	0.001612682

H	-5.138232679	-1.238997407	0.001471313
H	-5.138370857	1.238728242	0.001557095
H	-3.424505270	-3.424679482	0.000981076
H	3.424957624	3.424771308	0.001125422
N	-2.709195798	2.708811281	0.000034993
H	-3.424990034	3.424595964	0.001125255
H	3.424469357	-3.424851567	0.001097764

3.5. V

C	-2.530996724	3.258451774	0.485552699
C	-3.257870174	2.531560478	-0.485102392
C	-2.839369468	1.278862338	-0.848929648
C	-1.628460017	0.708017233	-0.332066496
C	-0.708013205	1.628307343	0.333334875
C	-1.278744388	2.839393379	0.850167476
As	-3.876060510	0.000067906	-1.904319507
C	-2.838793558	-1.278930007	-0.849766749
C	-1.628140441	-0.708133106	-0.332430677
C	-3.257116651	-2.531734945	-0.485992855
C	-2.530515146	-3.258316231	0.485311397
C	-1.278588148	-2.838905131	0.850689156
C	-0.707939172	-1.627656214	0.333695480
H	-2.945517455	-4.180001708	0.874373137
H	-4.177937737	-2.947513351	-0.876285318
H	-4.178986947	2.946989396	-0.874932067
H	-2.946066619	4.179954993	0.874853472
As	0.000214800	3.876159673	1.905334381
C	1.278872401	2.839400883	0.849830388
C	0.708122541	1.628583686	0.332657595
C	1.627607022	0.708027737	-0.332668385

C	2.838491432	1.278547119	-0.850769340
C	3.257606018	2.530836721	-0.486278999
C	2.531587332	3.257514814	0.485566397
C	1.627630241	-0.708061307	-0.332356152
C	2.838308108	-1.278608593	-0.850732789
As	3.874896365	-0.000122320	-1.906519626
C	0.708116323	-1.627949997	0.333273026
C	1.278587001	-2.839011498	0.850604199
C	2.531105981	-3.257423760	0.485988134
C	3.257098197	-2.531042530	-0.486305429
H	2.946993052	-4.178442755	0.875862630
As	0.000001938	-3.876144080	1.905787348
H	4.178030340	-2.946715121	-0.876609767
H	4.178812527	2.946101459	-0.876252562
H	2.947685597	4.178307705	0.875636989
H	-5.098766270	-0.000676020	-0.993514371
H	0.000193480	5.099101306	0.994809056
H	0.000051316	-5.098523357	0.994417449
H	5.097870621	-0.000273911	-0.995912156

3.6. VI

C	1.386639955	3.031292382	-0.000586219
C	2.870621488	2.870639374	0.000113737
C	0.726930115	1.747444776	-0.000174798
C	1.747456747	0.726935677	0.000485048
C	3.031299922	1.386648780	0.000715194
C	-0.684025030	1.732259392	0.000151473
C	-1.732491729	0.683776521	0.001278024
C	-1.747569699	-0.726807428	0.001460132
C	-0.726802354	-1.747558323	0.000695481

C	0.683770892	-1.732481931	0.000346447
C	1.732270465	-0.684030056	0.000731106
C	2.973696190	-1.334671718	0.000777053
C	1.334583175	-2.973959689	-0.000579753
C	2.802755415	-2.802947313	0.000013603
C	4.216258879	-0.666471517	0.001179944
C	4.241241439	0.714069488	0.001237732
H	5.176404614	1.258485908	0.001673959
H	5.134720402	-1.240847499	0.001173205
C	0.666412481	-4.216687345	-0.001731910
C	-0.713795583	-4.241302619	-0.001661434
C	-1.386291095	-3.031007608	-0.000245579
C	-2.870266106	-2.870283868	0.000351362
C	-3.031014940	-1.386299991	0.001228927
C	-4.241279797	-0.713811206	0.001184723
C	-4.216662250	0.666426660	0.001222026
C	-2.973964944	1.334592259	0.001018946
C	-2.802932380	2.802771286	0.000001460
C	-1.334662274	2.973690094	-0.000544697
C	-0.666456560	4.216283197	-0.001590537
C	0.714054433	4.241264767	-0.001537133
H	-1.240851840	5.134731940	-0.002484572
H	1.258492750	5.176415002	-0.002383561
H	-5.135047733	1.240761300	0.001176372
H	-5.176249254	-1.258400026	0.000564116
H	-1.258406673	-5.176258656	-0.002743308
H	1.240765525	-5.135060407	-0.002746198
H	3.333834293	3.334639876	0.876965854
H	-3.333581295	-3.334468935	0.876934673

H	-3.278027073	3.278787191	0.870966702
H	3.277800810	-3.278761476	0.871115618
H	3.334634652	3.333919007	-0.876692883
H	3.278448052	-3.277872598	-0.871214055
H	-3.334185429	-3.333388328	-0.876483403
H	-3.278528656	3.277543658	-0.871362875

3.7. VII

C	-2.853896217	1.356721146	0.808160301
C	-1.655979143	0.693260314	0.324709265
C	-0.693248469	1.655887835	-0.323988843
C	0.693262232	1.655899358	-0.323966925
C	1.356700229	2.853632832	-0.807865302
C	-1.655976778	-0.693257243	0.324715216
C	-0.693250608	-1.655881372	-0.323989822
C	0.693263127	-1.655892202	-0.323971443
C	1.656014847	-0.693250469	0.324694355
C	1.656016753	0.693251890	0.324691873
C	2.853918766	1.356697648	0.808136216
Si	2.946081505	2.945975519	0.000013215
C	3.869763220	0.688306542	1.496765849
C	3.869762510	-0.688306817	1.496768433
C	2.853920225	-1.356698588	0.808134418
Si	2.946087087	-2.945978297	0.000004543
C	1.356703340	-2.853626823	-0.807876102
C	-1.356700632	-2.853626319	-0.807891032
C	-0.688301814	-3.869175907	-1.496985329
C	0.688313721	-3.869185847	-1.496956287
H	1.236758400	-4.699859132	-1.923233175
H	-1.236756756	-4.699832664	-1.923303981

H	3.982652307	-3.982468416	-0.000270361
H	4.700595793	-1.236748130	1.922719710
H	4.700597500	1.236745446	1.922713826
H	3.982639891	3.982463876	-0.000251389
C	0.688315400	3.869189294	-1.496943029
C	-0.688297404	3.869176597	-1.496979415
C	-1.356695000	2.853629609	-0.807891055
Si	-2.946109620	2.945986207	-0.000024490
C	-3.869752558	0.688316391	1.496813291
C	-3.869749270	-0.688309884	1.496823671
C	-2.853894970	-1.356718668	0.808169706
Si	-2.946110295	-2.945992845	-0.000007594
H	-3.982699395	-3.982501903	-0.000276983
H	-4.700624260	-1.236759645	1.922749816
H	-4.700634429	1.236764996	1.922723009
H	-3.982698250	3.982487205	-0.000303273
H	-1.236749668	4.699821770	-1.923310874
H	1.236758679	4.699856696	-1.923220005

4. The Cartesian coordinates of atoms in Å for the dianions

4.1. I

C	2.084717979	3.679097241	0.000599491
C	0.724484538	4.166173427	-0.000017946
C	-0.294582403	3.242731641	-0.001012333
C	-0.094136252	1.839880309	-0.001284425
C	1.240603919	1.361924901	-0.000494898
C	2.286038046	2.318650505	0.000269322
O	3.519107679	1.663324624	0.000859026
C	3.242734231	0.294580838	0.000502893
C	1.839883555	0.094134701	-0.000073480

C	4.166178232	-0.724484404	0.000412665
C	3.679101025	-2.084717050	-0.000293946
H	2.919687581	4.369204520	0.001501669
H	0.517200312	5.229496732	0.000454817
H	5.229499459	-0.517192524	0.000905980
H	4.369207965	-2.919687431	-0.000647746
C	1.361928937	-1.240603900	-0.000294252
C	2.318654059	-2.286037595	-0.000519038
O	1.663327302	-3.519107208	-0.000816171
C	0.294582901	-3.242732182	-0.000454966
C	0.094136577	-1.839880853	-0.000213612
C	-0.724485955	-4.166173138	-0.000182566
C	-2.084718622	-3.679097179	0.000602752
H	-0.517202685	-5.229496823	-0.000554038
H	-2.919688197	-4.369204653	0.001130679
C	-1.240603561	-1.361925448	0.000088134
C	-2.286038056	-2.318650415	0.000691300
O	-3.519107882	-1.663324237	0.001043747
C	-3.242734332	-0.294580785	0.000358726
C	-1.839883265	-0.094135412	-0.000329530
C	-4.166178036	0.724484929	0.000406468
C	-3.679100436	2.084717573	-0.000329308
C	-2.318653554	2.286037358	-0.001031718
C	-1.361928526	1.240603336	-0.001193548
H	-5.229499216	0.517193649	0.001157697
H	-4.369206688	2.919688472	-0.000104656
O	-1.663326632	3.519106481	-0.001137189

4.2. II

C	-1.243739637	3.057617004	0.395800168
---	--------------	-------------	-------------

C	-3.057631751	1.243738914	-0.395824418
S	-4.199108535	0.000000377	-0.843100238
H	4.514489108	2.809806326	-0.395134955
H	2.809817149	4.514464542	0.395204964
C	3.057631894	1.243739015	-0.395825984
S	4.199108485	-0.000000421	-0.843100923
C	3.057631783	-1.243739038	-0.395824423
C	1.732871411	-0.718233679	-0.144367099
C	1.732871690	0.718233419	-0.144366273
C	3.477825755	2.539316128	-0.229620211
C	2.539325182	3.477808258	0.229647267
C	1.243740045	3.057616951	0.395799985
C	0.718234040	1.732866260	0.144293400
C	3.477826598	-2.539314509	-0.229612872
C	2.539323824	-3.477808787	0.229644623
C	1.243739641	-3.057616869	0.395799635
C	0.718233762	-1.732866243	0.144293949
H	2.809812582	-4.514467379	0.395191078
H	4.514492881	-2.809801040	-0.395113440
C	-0.718233853	1.732866132	0.144294670
C	-1.732871477	0.718233488	-0.144366746
C	-1.732871762	-0.718233622	-0.144366676
C	-0.718234166	-1.732866470	0.144292608
C	-1.243739961	-3.057617075	0.395798984
C	-2.539325007	-3.477808248	0.229646622
C	-3.477826077	-2.539315882	-0.229619224
C	-3.057632035	-1.243739055	-0.395825689
H	-4.514489849	-2.809805748	-0.395131741
H	-2.809816713	-4.514464614	0.395204024

S	-0.000000076	-4.199084218	0.843090917
S	0.000000117	4.199084182	0.843092434
C	-2.539323840	3.477808612	0.229644643
C	-3.477826308	2.539314568	-0.229613895
H	-2.809812841	4.514467101	0.395191528
H	-4.514492060	2.809801619	-0.395116695

4.3. III

C	-1.268403515	2.981268388	0.613451571
P	0.000006855	4.013545679	1.392882583
C	-0.719702493	1.700594503	0.222819813
C	0.719704348	1.700597074	0.222808309
C	1.268408869	2.981271204	0.613434576
C	-1.700577854	0.719705461	-0.222677219
C	-1.700578836	-0.719704013	-0.222680661
C	-0.719704039	-1.700596643	0.222811513
C	0.719702972	-1.700593909	0.222822597
C	1.700578569	-0.719705814	-0.222676701
C	1.700579912	0.719703783	-0.222680586
C	2.981216235	1.268404037	-0.613420238
C	2.981220320	-1.268407275	-0.613396360
P	4.013447061	-0.000007226	-1.392906530
C	3.402971185	2.548431148	-0.366229487
C	2.548419775	3.403017403	0.366150231
H	2.874256154	4.395755725	0.662717822
H	4.395703711	2.874245211	-0.662840388
C	3.402987707	-2.548421832	-0.366164970
C	2.548408512	-3.403026549	0.366160022
C	1.268403442	-2.981268757	0.613452127
P	-0.000006909	-4.013546802	1.392883088

C	-1.268409095	-2.981271178	0.613436348
C	-2.548418934	-3.403018866	0.366148516
C	-3.402974157	-2.548428573	-0.366222007
C	-2.981215680	-1.268403816	-0.613418866
P	-4.013444895	0.000006649	-1.392909080
C	-2.981219290	1.268407187	-0.613398321
C	-3.402985860	2.548422713	-0.366169992
C	-2.548410197	3.403024287	0.366163119
H	-4.395756695	2.874204901	-0.662686253
H	-2.874211891	4.395796291	0.662654525
H	-4.395715353	-2.874234199	-0.662813014
H	-2.874248598	-4.395763912	0.662699957
H	2.874204622	-4.395804369	0.662637919
H	4.395764940	-2.874198472	-0.662665539
H	-0.000005219	5.114618614	0.484321270
H	0.000003778	-5.114619445	0.484321403
H	-5.114571869	-0.000007370	-0.484412913
H	5.114572413	0.000008763	-0.484408182

4.4. IV

C	1.144297729	3.081463565	-0.079138339
C	0.708355205	1.717809427	-0.025350784
C	1.717824574	0.708349568	0.025048842
C	1.717821786	-0.708360518	0.025298777
C	3.081474605	-1.144298200	0.079046743
C	3.081473597	1.144295336	0.078935993
C	0.708356512	-1.717830650	-0.024740127
N	3.892068147	0.000005122	0.198191024
C	1.144299152	-3.081464960	-0.078826509
C	3.476654657	2.465117223	0.046804932

C	2.465112840	3.476656428	-0.046871636
C	2.465118939	-3.476645117	-0.046848861
C	3.476657743	-2.465113525	0.046881730
H	4.526549084	2.735204332	0.111788669
H	2.735190948	4.526563131	-0.111688299
H	2.735199229	-4.526529813	-0.111939728
H	4.526551224	-2.735198027	0.111824425
H	4.810261988	-0.000014690	-0.213467389
C	-0.708354849	1.717809104	-0.025357834
C	-1.144297264	3.081463522	-0.079140260
C	-1.717825021	0.708349124	0.025031120
C	-1.717822974	-0.708361205	0.025281012
C	-0.708357446	-1.717831046	-0.024747703
C	-3.081473325	1.144295253	0.078929528
C	-3.081475342	-1.144298989	0.079039127
C	-1.144299491	-3.081465385	-0.078829332
C	-3.476653736	2.465117551	0.046808201
C	-2.465112170	3.476656682	-0.046870750
C	-2.465118929	-3.476646165	-0.046849256
C	-3.476658071	-2.465114987	0.046882272
H	-4.526547450	2.735204754	0.111799991
H	-2.735189911	4.526563634	-0.111684168
H	-2.735198766	-4.526531317	-0.111935797
H	-4.526551086	-2.735200285	0.111830644
N	-3.892067728	0.000004885	0.198188242
H	-4.810264112	-0.000014142	-0.213464322
N	0.000000329	3.892061098	-0.198385301
N	0.000000070	-3.892042449	-0.198183829
H	-0.000000188	4.810242461	0.213310912

H	-0.000000498	-4.810270730	0.213398039
---	--------------	--------------	-------------

4.5. V

C	-2.563120187	3.352539634	0.437011455
---	--------------	-------------	-------------

C	-3.352559855	2.563105408	-0.436988673
---	--------------	-------------	--------------

C	-2.910219148	1.304497559	-0.743096512
---	--------------	-------------	--------------

C	-1.674961133	0.718976978	-0.275685525
---	--------------	-------------	--------------

C	-0.718977914	1.674962606	0.275643629
---	--------------	-------------	-------------

C	-1.304498945	2.910210633	0.743082093
---	--------------	-------------	-------------

As	-3.960643705	0.000001632	-1.741736416
----	--------------	-------------	--------------

C	-2.910214939	-1.304496543	-0.743103766
---	--------------	--------------	--------------

C	-1.674956357	-0.718977542	-0.275693650
---	--------------	--------------	--------------

C	-3.352558195	-2.563102469	-0.436993901
---	--------------	--------------	--------------

C	-2.563115997	-3.352541625	0.436998900
---	--------------	--------------	-------------

C	-1.304498431	-2.910209768	0.743079651
---	--------------	--------------	-------------

C	-0.718975515	-1.674961054	0.275642576
---	--------------	--------------	-------------

H	-2.922900794	-4.315314341	0.788415223
---	--------------	--------------	-------------

H	-4.315335466	-2.922886020	-0.788398280
---	--------------	--------------	--------------

H	-4.315331372	2.922895474	-0.788403031
---	--------------	-------------	--------------

H	-2.922913379	4.315302006	0.788448266
---	--------------	-------------	-------------

As	-0.000003990	3.960636815	1.741718430
----	--------------	-------------	-------------

C	1.304497068	2.910215455	0.743086601
---	-------------	-------------	-------------

C	0.718979367	1.674963450	0.275656470
---	-------------	-------------	-------------

C	1.674971658	0.718978517	-0.275655320
---	-------------	-------------	--------------

C	2.910219205	1.304501004	-0.743088701
---	-------------	-------------	--------------

C	3.352554999	2.563114679	-0.436995412
---	-------------	-------------	--------------

C	2.563116821	3.352546918	0.437009059
---	-------------	-------------	-------------

C	1.674978847	-0.718977119	-0.275641647
---	-------------	--------------	--------------

C	2.910225457	-1.304501341	-0.743076633
---	-------------	--------------	--------------

As	3.960626265	-0.000002152	-1.741741753
----	-------------	--------------	--------------

C	0.718981540	-1.674964509	0.275659732
C	1.304496975	-2.910217947	0.743088018
C	2.563120183	-3.352545808	0.437019675
C	3.352556781	-2.563117629	-0.436989416
H	2.922932930	-4.315285558	0.788498711
As	-0.000006151	-3.960638304	1.741716200
H	4.315304934	-2.922927828	-0.788446855
H	4.315322321	2.922907294	-0.788418679
H	2.922911908	4.315307560	0.788448801
H	-5.201697130	-0.000003521	-0.830618988
H	-0.000001561	5.201690325	0.830601836
H	-0.000006773	-5.201692268	0.830599920
H	5.201699678	0.000009399	-0.830652086

4.6. VI

C	1.361660489	3.031151632	-0.000715374
C	2.854060039	2.854060095	0.000452840
C	0.722261026	1.741736887	-0.001453957
C	1.741736427	0.722260710	-0.000741956
C	3.031150711	1.361659905	0.000557458
C	-0.722260968	1.741736792	-0.001670953
C	-1.741736513	0.722260735	-0.000820023
C	-1.741736129	-0.722260773	-0.000190707
C	-0.722260477	-1.741736724	-0.000573296
C	0.722261062	-1.741736693	-0.000963578
C	1.741736334	-0.722260971	-0.000706439
C	3.031150668	-1.361660410	-0.000013813
C	1.361660581	-3.031151314	-0.001146693
C	2.854060194	-2.854059944	-0.000894535
C	4.234705303	-0.712123576	0.001433161

C	4.234705150	0.712121689	0.001895892
H	5.164736777	1.275708328	0.003214848
H	5.164737138	-1.275711001	0.002168340
C	0.712122722	-4.234706498	-0.001234178
C	-0.712122736	-4.234706545	-0.000732475
C	-1.361660167	-3.031151215	-0.000272645
C	-2.854059706	-2.854059597	0.000740590
C	-3.031150307	-1.361659900	0.000892299
C	-4.234704929	-0.712122317	0.001901297
C	-4.234705476	0.712122948	0.001402169
C	-3.031151043	1.361660220	-0.000114368
C	-2.854060489	2.854059813	-0.001091116
C	-1.361660759	3.031151493	-0.001500852
C	-0.712122805	4.234706562	-0.001060437
C	0.712122534	4.234706659	-0.000558314
H	-1.275709569	5.164738772	-0.000629911
H	1.275708984	5.164738810	0.000348939
H	-5.164737079	1.275710392	0.002175744
H	-5.164736476	-1.275709420	0.002859896
H	-1.275709674	-5.164738809	-0.000479556
H	1.275709960	-5.164738622	-0.001351792
H	3.316949206	3.317657752	0.881001369
H	-3.317072529	-3.317728597	0.881187226
H	-3.317509234	3.318275524	0.878833079
H	3.317600328	-3.318240459	0.879001155
H	3.318425292	3.317717292	-0.879291312
H	3.317775315	-3.317132357	-0.881292199
H	-3.318302055	-3.317644256	-0.879105736
H	-3.317867119	3.317096988	-0.881460088

4.7. VII

C	2.816835186	-1.380539129	0.838652116
C	1.659480862	-0.699064975	0.316654864
C	0.705132933	-1.658475366	-0.353487217
C	-0.698103720	-1.661397413	-0.354063468
C	-1.366662605	-2.854917520	-0.796463953
C	1.656628323	0.706207549	0.316034089
C	0.697995284	1.661335239	-0.354093889
C	-0.705246050	1.658544176	-0.353444777
C	-1.659732937	0.699034916	0.316547255
C	-1.656880349	-0.706169416	0.315919411
C	-2.811604748	-1.392748386	0.837060008
Si	-3.087645337	-2.950320114	-0.128074527
C	-3.774880238	-0.696843260	1.572673000
C	-3.777491973	0.679959375	1.573609381
C	-2.817003300	1.380499937	0.838722659
Si	-3.099752748	2.937890602	-0.124852708
C	-1.378999173	2.849488972	-0.794884404
C	1.366768665	2.854688646	-0.796714479
C	0.681297263	3.880527147	-1.442602828
C	-0.698278094	3.878009377	-1.441504063
H	-1.250058595	4.734835787	-1.820709168
H	1.229350401	4.739539794	-1.822345192
H	-3.203955006	4.189604219	0.715987722
H	-4.608064907	1.219942674	2.022218140
H	-4.603363103	-1.240597808	2.020585787
H	-3.188127504	-4.203125057	0.711558892
C	-0.681164160	-3.880708535	-1.442378768
C	0.698407574	-3.877850031	-1.441694433

C	1.379098309	-2.849249766	-0.795154166
Si	3.100452044	-2.937378078	-0.126048791
C	3.776915307	-0.679987451	1.574135028
C	3.774318871	0.696861964	1.573185294
C	2.811439648	1.392795942	0.837000535
Si	3.088378208	2.949856135	-0.129242714
H	3.188661207	4.202958528	0.710283284
H	4.602731242	1.240633719	2.021327281
H	4.607326597	-1.220001191	2.023117932
H	3.204601344	-4.189426949	0.714571827
H	1.250297508	-4.734714562	-1.820726222
H	-1.229102233	-4.739699692	-1.822248739