Journal Name

ARTICLE TYPE

Cite this: DOI: 10.1039/xxxxxxxxxx

Supplementary Information: **Bicycloaromaticity and Baird-type bicycloaromaticity of dithienothiophene-bridged [34]octaphyrins**†

Rashid R. Valiev,[a,b] Heike Fliegl[c], Dage Sundholm*[a,d]

Received Date
Accepted Date

DOI: 10.1039/xxxxxxxxxx

www.rsc.org/journalname

Contents

[a] *Department of Chemistry, University of Helsinki, P.O.Box 55, FIN-00014 Helsinki, Finland*
[b] *Department of Optics and Spectroscopy, Tomsk State University, Tomsk, Lenina Avenue 36, Russian Federation*
[c] *Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, University of Oslo, P.O.Box 1033 Blindern, 0315 Oslo, Norway*
[d] *Centre for Advanced Study at the Norwegian Academy of Science and Letters, Drammensveien 78, N-0271 Oslo, Norway, Email:Dage.Sundholm@helsinki.fi*

† Electronic Supplementary Information (ESI) available: Cartesian coordinates of the optimized structures and NMR shielding constants. Additional streamline plots and current pathways. See DOI: 10.1039/b000000x/

Detailed current strengths

Current pathways in 1a and 2a

The small loop in **1a** sustains a ring current of 10.5 nA/T (10.0 nA/T). The corresponding values for **2a** are given in parenthesis. The current strength of the large loop is 22.0 nA/T (23.3 nA/T) and 10.5 nA/T (10.0 nA/T) passes the bridge.

The ring-current of the common path of the small and large loops is split at the two thiophenes into an outer pathway of 25.6 nA/T (30.3 nA/T) and an inner one of 5.5 nA/T (2.0 nA/T). At the thiophene between the two thiophene ring of the common loop of **2a**, the current strength of 11.6 nA/T along the outer branch is weaker than the current of 21.4 nA/T that passes via the inner pathway. At the pyrrolic rings of the common loop, a current of 18.6 nA/T (20.8 nA/T) passes the nitrogen moiety and 12.5 nA/T (11.5 nA/T) takes the outer route.

At the outer thiophene rings of the bridge, the ring current avoids the sulfur moiety, whereas at the thiophene in the middle of the bridge the current is almost equally split into a current of 5.5 nA/T (3.5 nA/T) that passes the sulfur atom and 4.9 nA/T (6.5 nA/T) along the other route.

The ring current of the large loop is divided at the pyrrolic rings into an inner pathway whose strength is 13.6 nA/T (15.3 nA/T) and a current of 8.4 nA/T (8.0 nA/T) that takes the outer route. At the thiophene moieties of the large loop, the current is divided into a weaker pathway of 5.5 nA/T (0.0 nA/T) that passes the sulfur atoms, whereas the current strength of the outer pathway is 16.5 nA/T (23.3 nA/T). For **2a**, the current pathway of the large loop is almost equally split at the thiophene ring in the middle. The strength of the current via the sulfur atom is 11.0 nA/T and a current of 12.3 nA/T takes the inner pathway.

Current pathways in the triplet state of $\mathbf{1a}^{2+}$

The large loop of $\mathbf{1a}^{2+}$ sustains a very weak ring current of 3.2 nA/T as compared to 22.0 nA/T for **1a**. The thiophene and

pyrrolic rings of the large loop sustain local ring currents of 6.8 nA/T and 1.0 nA/T, respectively. The current strength of the small loop is 29.0 nA/T for $\mathbf{1a}^{2+}$, which is almost three times stronger than for **1a**. The current flow across the bridge is split at the thiophene rings. However, the current flow avoids the sulfur atoms leading to very weak currents of 0.2 nA/T and 3.5 nA/T via them. The current density flows mainly along the inner pathway via the nitrogen moiety of the pyrrolic rings of the small ring. At the thiophene rings of the small loop, the current strength along the outer route is 23.3 nA/T and a current with a strength of 8.7 nA/T flows via the sulfur moiety. The large loop of the doubly charge $\mathbf{1a}^{2+}$ is practically nonaromatic with aromatic thiophene rings. The pyrrolic rings of the large loop are almost nonaromatic.

Current pathways in the triplet state of $\mathbf{2a}^{2+}$

The small loop in $\mathbf{2a}^{2+}$ sustains a ring current of 15.8 nA/T (10.0 nA/T) and for the large loop is it is 19.0 nA/T (23.3 nA/T). The values in parenthesis are for neutral **2a**. The ring current of the common path of the two loops splits at the two thiophenes into an outer pathway of 31.9 nA/T (30.3 nA/T) and an inner one of 3.5 nA/T (2.0 nA/T). At the middle thiophene ring of the common loop, a current with a strength of 10.9 nA/T (11.6 nA/T) passes via the outer pathway and 24.5 nA/T (21.4 nA/T) takes the inner route. At the pyrrolic rings of the common loop, a current with a strength of 26.1 nA/T (20.8 nA/T) passes the the nitrogen moiety of the pyrrolic rings of the common part of the loops and a current of 9.3 nA/T (11.5 nA/T) passes the β carbons. The current strengths via the sulfur moieties of the thiophene rings of the bridge are 3.1 nA/T (0.2 nA/T), 10.6 nA/T (3.5 nA/T) and 3.1 nA/T (0.2 nA/T).

The ring current splits at the pyrrolic rings of the large loop into an inner pathway whose strength is 15.2 nA/T (15.3 nA/T) and 3.8 nA/T (8.0 nA/T) takes the outer route. The ring current splits at the thiophene rings of the large loop into a weaker pathway of 5.7 nA/T (0.0 nA/T) that passes the sulfur atoms and along the outer pathway the current strength is 13.3 nA/T (23.3 nA/T). At the thiophene ring in the middle of the large loop, the strength of the current via the sulfur atom is 11.5 nA/T (11.0 nA/T) and a current of 7.5 nA/T (12.3 nA/T) takes the inner route.

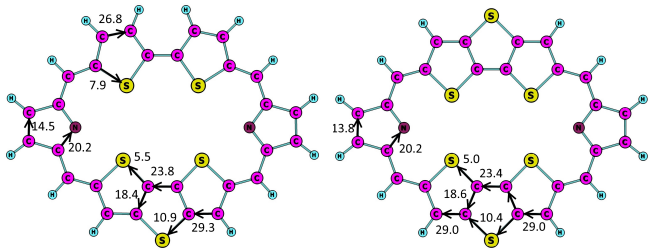
Current pathways in the doublet state of $\mathbf{1a}^{1+}$ and $\mathbf{2a}^{1+}$

The small loop of $\mathbf{1a}^{1+}$ sustains a paratropic ring current of -8.0 nA/T (-11.0 nA/T). The corresponding current strengths for $\mathbf{2a}^{1+}$ are given in parenthesis. The current strength of the large loop is -2.4 nA/T (-5.2 nA/T) and -5.9 nA/T (-5.8 nA/T) passes the bridge. The two thiophene rings of the large loop of $\mathbf{1a}^{1+}$ sustain a local diatropic ring current of 3.9 nA/T. The thiophene rings of the common part of the large and small loops of molecule $\mathbf{1a}^{1+}$ sustain local diatropic ring currents of 1.2 nA/T.

For $\mathbf{2a}^{1+}$, the global paratropic ring current of the large loop takes the inner route at the three thiophene rings and a diatropic current of 3.0 nA/T passes along the outer part of the three thiophene rings. The thiophene ring in the middle sustains a local diatropic ring current of 2.8 nA/T. Similar current pathway pattern is obtained for the bridges of $\mathbf{1a}^{1+}$ and $\mathbf{2a}^{1+}$ and for the three thiophene rings of the common part of the two loops of molecule $\mathbf{2a}^{1+}$. The global paratropic ring current passes on the inside of the three thiophene rings. For $\mathbf{1a}^{1+}$, a diatropic current of 1.3 nA/T (1.0 nA/T) passes along the outer side of the bridge and the thiophene in the middle sustains a local diatropic ring current of 2.8 nA/T (2.0 nA/T). Current strengths for $\mathbf{2a}^{1+}$ are given in parenthesis. In $\mathbf{2a}^{1+}$, a diatropic current of 1.2 nA/T flow along the outer part of the three thiophenes of the common part of the two loops. The thiophene ring in the middle sustains a local diatropic ring current of 2.0 nA/T.

Current pathways in 1b and 2b

The singlet states of the neutral **1b** and **2b** rings are aromatic sustaining a ring current strength of 34.7 nA/T (34.0 nA/T). The current strengths for **2b** are given in parenthesis. At the thiophenes the ring current splits into a outer pathway of 29.3 nA/T (29.0 nA/T) and the current strength of the inner pathway is 5.5 nA/T (5.0 nA/T). At the pyrrolic rings, the ring current is split into two almost equally strong pathways. The current strength of the inner one is 20.2 nA/T (20.2 nA/T) and a current of 14.5 (13.8 nA/T) takes the outer route. The ring current strength passing the sulfur bridge is 10.9 nA/T (10.4 nA/T) and 23.8 nA/T (23.4 nA/T) passes via the C–C link. At the thiophene rings of **1b** that are connected with a C–C bond, a current of 26.8 nA/T takes the outer pathway and 7.9 nA/T the inner one.

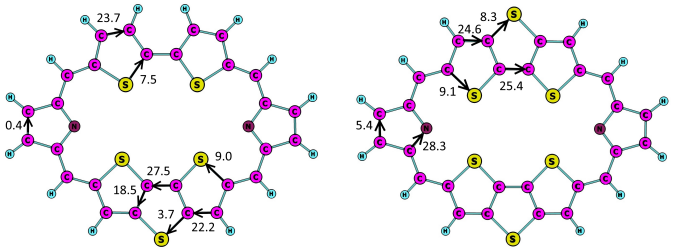


(a) **1b** (b) **2b**

Fig. 1 The strengths (in nA/T) of the current pathways of **1b** and **2b** calculated at the B3LYP/def2-TZVP level of theory.

Current pathways in the triplet state of $\mathbf{1b}^{2+}$ and $\mathbf{2b}^{2+}$

The triplet states of the $\mathbf{1b}^{2+}$ and $\mathbf{2b}^{2+}$ dications are aromatic sustaining a ring current strength of 31.2 nA/T (33.7 nA/T). The current strengths for $\mathbf{2b}^{2+}$ are given in parenthesis. At the thiophenes the ring current splits into a outer pathway of 22.2 nA/T (24.6 nA/T) and the current strength of the inner pathway is 9.0 nA/T (9.1 nA/T). At the pyrrolic rings, the main part of the ring current of 30.8 nA/T (28.3 nA/T) passes the inner nitrogen moiety and only 0.4 nA/T (5.4 nA/T) takes the outer route. The ring current strength passing the sulfur bridge is 3.7 nA/T (8.3 nA/T) and 27.5 nA/T (25.4 nA/T) passes via the C–C link. At the thiophene rings of $\mathbf{1b}^{2+}$ that are connected with a C–C bond, a current of 23.7 nA/T takes the outer pathway and a current of 7.5 nA/T flows via the inner one.

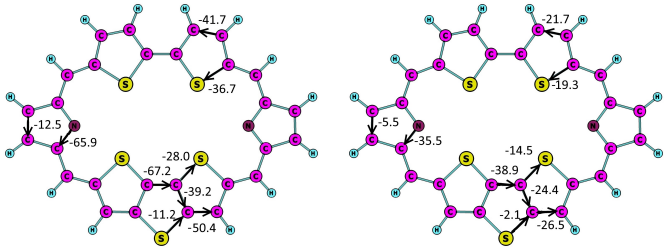


($\mathbf{1b}^{2+}$) ($\mathbf{2b}^{2+}$)

Fig. 2 The strengths (in nA/T) of the current pathways of the triplet state of the $\mathbf{1b}^{2+}$ and $\mathbf{2b}^{2+}$ dications calculated at the B3LYP/def2-SVP level of theory.

Current pathways in the singlet state of $\mathbf{1b}^{2+}$

The singlet state of the $\mathbf{1b}^{2+}$ dication is strongly antiaromatic sustaining a net paratropic ring current of -78.4 nA/T at the B3LYP level and -41.0 nA/T when using the BHLYP functional. The ring current splits almost equally at the thiophene rings that are connected with only one bond. At the BHLYP level -21.7 nA/T (-41.7 nA/T) passes the β carbons and -19.3 nA/T (-36.7 nA/T) passes the sulfur moiety. For the two corresponding thiophene ring on the other side of the molecule the ring current splits into a current of -26.5 nA/T (-50.4 nA/T) that passes the β carbons and a weaker current of -14.5 nA/T (-28.0 nA/T) that passes the sulfur moiety. A very weak current of -2.1 nA/T (-11.2 nA/T) passes the sulfur bridge between the two thiophene rings, whereas the current strength passing the C–C bond is -38.9 nA/T (-67.2 nA/T). At the pyrrole rings, a current of -35.5 nA/T (-65.9 nA/T) takes the inner route and -5.5 nA/T (-12.5 nA/T) passes via the β carbons. The corresponding current strengths obtained in the B3LYP calculation are given in parenthesis. The current strengths passing selected bonds of the $\mathbf{1b}^{2+}$ dication calculated at the B3LYP and BHLYP levels of theory are shown in Figures 3a and 3b, respectively.



(a) (b)

Fig. 3 The strengths (in nA/T) of the current pathways of the singlet state of the $\mathbf{1b}^{2+}$ dication calculated at (a) the B3LYP/def2-TZVP and (b) BHLYP/def2-TZVP levels of theory.

Cartesian coordinates

Singlet state of molecule 1a, B3LYP

The atomic coordinates in atomic units optimized at the B3LYP/def2-TZVP level.

-3.10028892844583	-12.93566570272522	2.27398606757783	C
2.69071735246707	-13.02380914955854	2.27478121401825	C
-1.51195020033156	-10.80974828874568	2.24978829909414	C
1.16784091784550	-10.85050492229695	2.25208842168768	C
3.05219510732037	-8.15149284601670	2.06653990465861	S
-3.31295618746844	-8.05502817153589	2.05557176052937	S
-6.14619169040381	-9.74473832395847	1.92395210956993	C
-5.63276761214326	-12.34840259335299	2.08519029805060	C
5.83291862248256	-9.92640208052412	1.93617414656259	C
5.24019820255374	-12.51354117897337	2.09108660297441	C
8.27526194331969	-8.98042157282645	1.54390065343719	C
9.11588590242386	-6.50508580854760	1.34163441056666	C
-8.55769176247676	-8.72567530699931	1.52391527678096	C
-9.32125160139645	-6.22630207812186	1.31213156788043	C
-7.86411970184343	-4.16500725572295	1.79515354175168	N
7.72150282860667	-4.40115334786210	1.82627494809795	N
-9.23291697094793	-2.12065539463759	1.16029587380900	C
-11.70583660978057	-2.88270437309101	0.20546113274386	C
-11.78034794559942	-5.43620475594411	0.37456460429456	C
9.15526867653499	-2.39829545999570	1.20252771732426	C
11.60683939251983	-3.23352970652142	0.25389300904989	C
11.60148249222122	-5.78864424226594	0.41476225446154	C
-8.20667083178519	0.35929971735003	1.39472170800333	C
-5.82833522516196	0.76293817016103	2.54312833784927	C
8.20543723488093	0.11161104482791	1.43943315626692	C
5.83462937348717	0.58616278396906	2.57615363959925	C
-3.59382424276220	-1.66890337861343	2.96310156030823	S
3.52448312079314	-1.77681073789143	2.98102906338885	S
-1.30709712423941	0.54187651624394	3.66573382573243	C
-4.82505593807856	3.13963938833036	3.22250258364224	C
-2.29630117373711	3.02087079020634	3.81192853734300	C
1.30230497400759	0.50216442537547	3.67310180657898	C
2.36561139709561	2.94987626006672	3.82642558988254	C
4.90044266540826	2.99175291593268	3.25289567684678	C
0.06905137676836	5.31729155170358	4.17949824031623	S
-10.02680598813049	-10.12854550496115	1.23894238880308	H
9.70133868250565	-10.42688853349760	1.25809223596127	H
-9.32714268672681	2.53093067414912	0.13821472031152	C
9.40027795690510	2.25092698214804	0.19594137624359	C
-13.17047839639294	-1.66378728591772	-0.50248794051451	H
-13.30987961296536	-6.67977257414170	-0.15196211671854	H
13.11092049818562	-2.05825401261381	-0.44532308536248	H
13.09355336548645	-7.07741338905640	-0.11063234779715	H
6.69469423232244	-13.94865632942735	2.03774542538230	H
-7.13017414524564	-13.73867655434242	2.03219409093297	H
-5.91774729182898	4.84976742503150	3.12570546297949	H
6.04550657563196	4.66776804297821	3.16476214326273	H
7.96839494179131	4.03048331106207	-0.85701831546447	N
-7.83445325835841	4.26238581375128	-0.91056735210703	N
9.56548059678554	5.78438532254660	-1.88344154546305	C
-9.37037824287364	6.05959668689271	-1.95531927374969	C
-11.98487179055378	3.19681113098424	-0.22257543109530	C
-12.00393930820184	5.41267326772428	-1.51233349579432	C
12.07949412456530	2.83660988103399	-0.14426543567952	C
12.17500311181042	5.05634154365571	-1.42420313149574	C
-13.59246179398482	2.18352033581227	0.50819084605806	H
-13.62498221604581	6.51041246865866	-2.08732440728732	H

13.83271944311494	6.10671752844456	−1.98298676030182	H
13.65033966268319	1.77158906598322	0.59304676047323	H
8.71034036515868	7.88868710882258	−3.14286979928628	C
−8.44386416962126	8.13206431382154	−3.21695518274963	C
6.19269293640939	8.66795160416335	−3.58585850492819	C
−5.90130990737405	8.83684016083153	−3.64193934834204	C
3.41799632449680	7.13782553440551	−2.62456158948523	S
−3.17953747466310	7.23441669617717	−2.64782140791473	S
1.51309268353227	9.46267369918029	−3.99639569139384	C
5.58292984552287	10.87411356296525	−4.90014995555567	C
3.01515252931575	11.31554449764987	−5.12963056190329	C
−1.19769714733985	9.49965837433333	−4.01040420858893	C
−2.63676631081630	11.38794177920605	−5.16662079175641	C
−5.21788751511045	11.01889030918428	−4.96023238213747	C
−6.61869950990167	12.28664847808606	−5.74012109896079	H
7.02588722179577	12.10597372177070	−5.66049662730350	H
−9.82300240703476	9.43289687833272	−3.99970170775937	H
10.13300400018944	9.15245065774841	−3.90827411464642	H
−2.38944306337529	−14.84532990042524	2.38691802845485	H
1.92188638454584	−14.91122483385068	2.38194357571342	H
−1.81195702625161	12.98156754422161	−6.13540373886915	H
2.24430594590764	12.93672762903897	−6.09714724484418	H

Triplet state of molecule $1a^{2+}$, B3LYP

The atomic coordinates in atomic units optimized at the B3LYP/def2-TZVP level.

−3.08626248934889	−12.90874443286032	2.14624522369326	C
2.68437427843478	−12.99525645657008	2.17731323299637	C
−1.49803505915935	−10.75597510306172	2.08241942821429	C
1.16202328484342	−10.79592438489373	2.09487798469863	C
3.04873487801731	−8.09653942621487	1.89747258026675	S
−3.30102043341148	−8.00087643007743	1.87244935249695	S
−6.11355658529807	−9.70622920225866	1.80489099661757	C
−5.60480668742057	−12.32981462633080	1.98146086926626	C
5.80947179674108	−9.88560015022050	1.85841641230511	C
5.22046370049343	−12.49244520448170	2.03542628977493	C
8.27530153822660	−8.97035716059011	1.55123770984751	C
9.13806251471163	−6.49786334678354	1.37549643969029	C
−8.54799872782968	−8.71627128715098	1.47751520694491	C
−9.33338806469519	−6.21841338832035	1.30091461740526	C
−7.85179407953592	−4.15872319854320	1.72733113246998	N
7.71635036324581	−4.39270063129161	1.78181512518171	N
−9.27213388383455	−2.12762262741482	1.20846690423376	C
−11.81774601704232	−2.89000287532478	0.39411613844552	C
−11.86679955992577	−5.43220422605720	0.52308723423320	C
9.20287653750686	−2.40713441684798	1.27088556121766	C
11.73208124103846	−3.24978475064569	0.48430956831817	C
11.70180498738180	−5.79189397672775	0.62066228113396	C
−8.23367305860914	0.36158710225720	1.40725322552239	C
−5.83226538794653	0.76325987108280	2.51844497288495	C
8.23632003942680	0.11245010564905	1.45150851775531	C
5.83829573438872	0.58736572810002	2.54752458891602	C
−3.56687989372021	−1.64426884575812	2.79453724375645	S
3.49995832092768	−1.75016122541215	2.80917200754905	S
−1.30772868049907	0.57779498780124	3.48657687121146	C
−4.85407044878153	3.14473566135971	3.22959877831925	C
−2.29208031568269	3.04664603524378	3.72813909591517	C
1.30550489316150	0.53840978142353	3.49273446738413	C
2.36275227353096	2.97587018809445	3.73976634218771	C
4.93031800011441	2.99603720491338	3.25474800395616	C
0.06977676825525	5.32957968844410	4.16186247974175	S

-10.01702372381759	-10.12904980270449	1.25934511129765	H
9.70295295845655	-10.42746157375805	1.35076605579110	H
-9.36992138312787	2.52477311623103	0.17536120080932	C
9.44050118656230	2.23528385044039	0.21902568558227	C
-13.33287704215953	-1.66546066866465	-0.18110173486483	H
-13.41804441649164	-6.68179811872591	0.08794355000098	H
13.29073387370601	-2.07473037020462	-0.07771096045040	H
13.21844489787898	-7.08959584664943	0.20467123186048	H
6.67842147655571	-13.92361356577166	2.04247837551199	H
-7.10497855329046	-13.71665285729499	1.97108764550274	H
-5.99887812810992	4.82355051646860	3.29104087305766	H
6.12533924184454	4.63940111684825	3.32316521513948	H
7.96304065795245	4.00186932691400	-0.83248727917239	N
-7.83659364427942	4.24236287548266	-0.87196090927085	N
9.54297327818238	5.75193321027504	-1.87255446855176	C
-9.36001177013175	6.04615129902173	-1.91066231628843	C
-12.01333651324380	3.21220152209542	-0.18692991500656	C
-12.00101401349772	5.43293825380340	-1.46537339823934	C
12.10457959302026	2.83722187517646	-0.14475051652910	C
12.16327432037395	5.05618596288411	-1.42484409780842	C
-13.63900818418850	2.23186975771184	0.54520262991796	H
-13.60736676507194	6.55032243568272	-2.03979737270398	H
13.80461880507277	6.12126447265994	-1.99985764665770	H
13.69865474347274	1.80740342126039	0.58880359450455	H
8.66796988541212	7.84536747868978	-3.16217068674477	C
-8.41706236821357	8.11234911302698	-3.19214424781015	C
6.16014605202437	8.61265468866779	-3.61610588768132	C
-5.88299140865998	8.80144069099471	-3.63782660406696	C
3.38391188889796	7.08694035826507	-2.66250394205751	S
-3.16036360437156	7.18869437674807	-2.67597311784200	S
1.50673360847841	9.41528513931845	-4.04167717807186	C
5.56826461097423	10.82439979843557	-4.94472709790782	C
3.00778652312705	11.27058352192114	-5.18303756946245	C
-1.20561661587135	9.45809620512852	-4.04643153552164	C
-2.64330585820352	11.36007226438170	-5.19080001319856	C
-5.21821925367069	10.99411960873265	-4.96143679594886	C
-6.62480201518285	12.26645346796628	-5.72137129421453	H
7.01678339205006	12.05090105487304	-5.70126608261665	H
-9.79609840046352	9.42242212348879	-3.95834008087718	H
10.09014789858857	9.10876458421280	-3.92791083689091	H
-2.37143921830782	-14.81415941477937	2.28454141578161	H
1.91149783017265	-14.87804694139478	2.31321266369535	H
-1.82618141737030	12.95721856614710	-6.15831795782105	H
2.24412579721570	12.89114412546259	-6.15525058872677	H

Triplet state of molecule 1a^{2+}, M06-2X

The atomic coordinates in atomic units optimized at the M06-2X/def2-TZVP level.

-3.04251839966629	-12.80339511970753	2.13532569867154	C
2.64267402403316	-12.88915020079915	2.15843371447337	C
-1.49063869404483	-10.62562744676369	2.08492112417366	C
1.15757033525934	-10.66562724761993	2.09481565500603	C
3.06202498597465	-8.00406482252281	1.88561713853961	S
-3.31206121629830	-7.90763902363725	1.86323062641710	S
-6.06879585537951	-9.63966063475966	1.75823181319969	C
-5.55820854939264	-12.25192303851044	1.93928653116502	C
5.76601712125950	-9.81832536784206	1.80399375814721	C
5.17532121897890	-12.41393211744651	1.98205561390212	C
8.25656596420998	-8.93828079046268	1.44614295351543	C
9.09525210382184	-6.49364341606580	1.29587493273701	C
-8.52843544605130	-8.68477710407418	1.37881558681830	C

-9.28943285658059	-6.21524845661264	1.22314363809829	C
-7.76640704740021	-4.16602280796391	1.68774843448977	N
7.63347154693133	-4.39617789929797	1.74212516416544	N
-9.15064932982303	-2.15296344395293	1.19765509583203	C
-11.71035170717804	-2.85308677803975	0.34325319901020	C
-11.80375505537094	-5.38244299302232	0.43705536541809	C
9.08546820067651	-2.42841808872435	1.26304762181693	C
11.63104164147523	-3.21159235415925	0.43757466935668	C
11.64270298034699	-5.74225365127607	0.53547880738025	C
-8.12635280003239	0.36005628504403	1.46080007217355	C
-5.77847615096159	0.76491805686744	2.59896164144136	C
8.13122561893069	0.11446398607379	1.50179259385502	C
5.78065752090550	0.59116293988463	2.62198878938016	C
-3.53847217746888	-1.62845218870742	2.99991189790613	S
3.46820318350070	-1.73199825262156	3.00368339428495	S
-1.30443520603119	0.60043726685104	3.65729739288053	C
-4.81083733602158	3.17561865515528	3.26400771533106	C
-2.27516885994853	3.08203678315971	3.81205299726806	C
1.29976225314116	0.56101466711879	3.66170501281619	C
2.34459177754591	3.01004831205805	3.82163303362785	C
4.88761854403474	3.02551546874268	3.28678703649686	C
0.07066593695897	5.36100022377230	4.20319252104641	S
-9.97150372633521	-10.11332062818950	1.10648773362569	H
9.65805511044367	-10.41024722672443	1.18822124311120	H
-9.28387265254836	2.52221014751660	0.23598649007872	C
9.35448222917713	2.23171464844810	0.27737191071719	C
-13.18589640342676	-1.58545156074631	-0.24332549066598	H
-13.36176582844544	-6.60936341269793	-0.03375982310562	H
13.15394503804073	-1.99468736247112	-0.13408438697097	H
13.16617204995445	-7.01859206598670	0.08350070060352	H
6.62869424410627	-13.84866657373710	1.96122368989279	H
-7.05406708039747	-13.64202422688144	1.90538699116517	H
-5.96279426447213	4.85292995686500	3.25242447229480	H
6.09024383846819	4.66670743128197	3.28513784148069	H
7.89470581315927	3.97440513526726	-0.79106022467207	N
-7.76954555617011	4.20612351979175	-0.83729258269825	N
9.49322860863044	5.70690057658707	-1.82953863933621	C
-9.31330755646812	5.99611253265985	-1.87734188720664	C
-11.93401579604239	3.19492314137452	-0.08132871930125	C
-11.94179972813886	5.38902243941631	-1.38910294780311	C
12.02441865841219	2.81541693621220	-0.04917092289896	C
12.10174186544258	5.01329403669397	-1.34824847859973	C
-13.54420545984630	2.23161460331620	0.70607805126515	H
-13.55261544016034	6.50614338986776	-1.94937537019846	H
13.74749090241813	6.07828836566717	-1.90856591723482	H
13.60475551219985	1.79935300370211	0.73147945424262	H
8.63507345433250	7.77524538598340	-3.14043451910313	C
-8.38950935791331	8.03319388731387	-3.18147674575873	C
6.12065732544319	8.53302263346352	-3.61369205141430	C
-5.84577002097833	8.71422277504828	-3.64761293123319	C
3.35901013433115	7.04763759970977	-2.65000311736046	S
-3.13803489158265	7.14510150671483	-2.67027663355578	S
1.51590892179327	9.33148239786937	-4.06589481290094	C
5.55898403816586	10.70769422804816	-4.97964428363813	C
2.99195185189315	11.15685036804587	-5.23727761050049	C
-1.21718901022221	9.37306522849379	-4.07392465987436	C
-2.62982853972473	11.24100821145882	-5.25163880899645	C
-5.21315932433816	10.86912836564298	-5.00815477573889	C
-6.63350695688840	12.11387007938541	-5.78723240897690	H
7.02110458120865	11.90798592356149	-5.75129777799596	H
-9.76640869867678	9.33792520247650	-3.96162940881066	H
10.05529076379538	9.03374640900303	-3.91903002231896	H

-2.30095889940739	-14.69755326214581	2.28284277055452	H
1.84335437049924	-14.75996340705636	2.30164341604385	H
-1.81075644862321	12.81669293761755	-6.25147151147707	H
2.22540405855594	12.75526732199471	-6.24253853557124	H

Singlet state of molecule 2a, B3LYP

The atomic coordinates in atomic units optimized at the B3LYP/def2-TZVP level.

-0.22505860485858	-14.49219696920741	1.01616677879888	S
-2.56137779507116	-12.17918063131463	1.57404750402780	C
2.17782231825665	-12.25173303642641	1.58734013631459	C
-1.46622149644384	-9.84862068947643	2.26552636569473	C
1.15066193127675	-9.88869473731005	2.27289719704860	C
3.41857590251832	-7.60043440889082	2.61049381787903	S
-3.66483616716722	-7.49198370367452	2.59059281130214	S
-6.10098422953973	-9.56636440258317	1.73569362988835	C
-5.16969171461758	-12.03429685007448	1.30765819709107	C
5.79481506331449	-9.74854819615427	1.76915659404149	C
4.79080958954889	-12.18682249572214	1.33556344844902	C
8.28622919397094	-8.95072759987417	1.35904297913889	C
9.19937389237145	-6.47960785035956	1.38244660419942	C
-8.56440296231455	-8.69265476571620	1.31142756939440	C
-9.40154656885636	-6.19475121122660	1.32963993359878	C
-7.98155734243273	-4.14781656656261	1.98611440585388	N
7.83896224842548	-4.39011217058959	2.03106211694625	N
-9.33093188820646	-2.07313947009039	1.38328158191313	C
-11.77518604378837	-2.80838906012763	0.33241150698270	C
-11.83304175330530	-5.36754138625720	0.35761151184201	C
9.25483004311445	-2.35773768185982	1.43661076676653	C
11.68149067204005	-3.16754166655448	0.39982338111948	C
11.66072127821824	-5.72728142878811	0.42481472664329	C
-8.31630400938293	0.41503979161344	1.60532150143551	C
-5.89149527985294	0.88393032950364	2.65302013539437	C
8.31569470483150	0.16036965725073	1.65334478035978	C
5.90035300079800	0.70335506019416	2.68707789888686	C
-3.61636985796089	-1.50803098812639	3.01164579753832	S
3.55093593564863	-1.61777841324840	3.03220586165104	S
-1.30828197686681	0.70372360015262	3.61362018978412	C
-4.86436684274204	3.27512798947929	3.25345926510413	C
-2.30728379427700	3.17773910213479	3.74933665907546	C
1.30825558144852	0.66366297536849	3.62114623443437	C
2.38174245737038	3.10592991409366	3.76294081371781	C
4.94346263694229	3.12488408054202	3.28199701639044	C
0.07212496347683	5.47651613370768	4.05931229313603	S
-9.92853482252057	-10.10719818953324	0.72795718308690	H
9.60967798220886	-10.40641624369125	0.78307253848517	H
-9.49347763539938	2.55800486203847	0.32707984363898	C
9.56541615915237	2.26629580563688	0.38247035934866	C
-13.22408451343043	-1.56411789692109	-0.36510874730859	H
-13.33341529819937	-6.58929640294865	-0.28972919500725	H
13.17189575989148	-1.96827735717614	-0.28900607119591	H
13.12671001811223	-6.99445868177383	-0.21392708163625	H
5.96561043578115	-13.75628655226227	0.76323047774193	H
-6.38878361117054	-13.56712801778253	0.72873280773703	H
-5.96367366920325	4.98283808323341	3.17291564600511	H
6.09507787607566	4.79805883931704	3.20821527922497	H
8.15144963146350	3.96772452219682	-0.79572735620762	N
-8.02125314968222	4.21493284160997	-0.84304336037572	N
9.73209095890956	5.70652466376734	-1.87556182291946	C
-9.54157426584741	6.00105764366270	-1.93224914380490	C
-12.14881764363661	3.26835719555957	0.01783197390735	C

-12.16904509569115	5.42652371725649	-1.37599950425565	C
12.24299465705977	2.89519151474158	0.08909761427339	C
12.33743151535050	5.05168314168432	-1.30426580454854	C
-13.75408970096643	2.32001855951080	0.83838446372084	H
-13.79221485555853	6.52318882797619	-1.94622197964545	H
13.99677050723532	6.09785394252207	-1.86514723791422	H
13.81363833179063	1.89847514224863	0.91924522418487	H
8.75653472990558	7.68636987920911	-3.25529996557298	C
-8.49784839056960	7.94987211165726	-3.30626389061326	C
6.14919964283876	8.15848504777117	-3.64641785851609	C
-5.87504084472966	8.34209802604144	-3.68195286905619	C
3.73374603049482	6.23088895385179	-2.39286467988754	S
-3.52703430346512	6.34179055913609	-2.41433680736144	S
1.45954927648680	8.18100741224621	-3.68090561950907	C
5.15544030622483	10.19751260532546	-5.00671568048712	C
2.51861438251857	10.21147730195675	-5.02563585443310	C
-1.18675108604963	8.22143128920264	-3.68872710878516	C
-2.17537304808299	10.28314273485143	-5.03954171619149	C
-4.81147135397357	10.34969037354765	-5.03622031384425	C
0.20525450480561	12.19871022473502	-6.32755331251054	S
-5.95517553787242	11.77537870345732	-5.94824175178351	H
6.34753425052367	11.58754818662792	-5.91175260339452	H
-9.75052878635840	9.32250658803053	-4.17126153231819	H
10.05562756969034	9.02024778765412	-4.11240655411376	H

Triplet state of molecule $2a^{2+}$, B3LYP

The atomic coordinates in atomic units optimized at the B3LYP/def2-TZVP level.

-0.22416765752301	-14.36541572692562	1.50127337277326	S
-2.53842010516387	-12.00616516610899	1.14634976072437	C
2.16295343231120	-12.07792670549469	1.15931822366982	C
-1.45357192912930	-9.59205405701518	0.71021645868145	C
1.15473073498609	-9.63182551093118	0.71766017545187	C
3.42999785535451	-7.33577817571538	0.54266858507678	S
-3.65658721863611	-7.22766569119979	0.52256677897236	S
-6.08210353936069	-9.41028729080799	1.06552261717065	C
-5.15185261476199	-11.90935590902823	1.30366571665095	C
5.78462976743726	-9.59154734581261	1.09848956743563	C
4.77725674693065	-12.06106541290819	1.33069603593609	C
8.34710628497598	-8.90705016992090	1.27163117688119	C
9.29383237654569	-6.46092780918133	1.38302933641120	C
-8.62333282929709	-8.64771591583754	1.22438147490815	C
-9.49527712965413	-6.17362930745461	1.32922023478783	C
-7.94947736224036	-4.11156868512125	1.59554658371869	N
7.81063959863348	-4.35241277576700	1.64242500229548	N
-9.41942416391716	-2.06920360895739	1.45121372006524	C
-12.07264679012876	-2.80524161244573	1.07498843504856	C
-12.11227233531354	-5.35772493390786	1.08159237999690	C
9.34348487831840	-2.35609880015728	1.50713057793883	C
11.97481208532926	-3.17321107754303	1.14445893771576	C
11.93603105398001	-5.72573868384983	1.15082112118304	C
-8.34036534719316	0.42379663746865	1.62295618376658	C
-5.88992157748309	0.84333271264288	2.63434924440368	C
8.34063545900190	0.16894860963484	1.67455752845685	C
5.89841909387749	0.66309967194305	2.67201296022901	C
-3.61743241226889	-1.56735561553545	2.94309733855699	S
3.55129124714712	-1.67706209047671	2.96619444547035	S
-1.31716152601095	0.63601775319102	3.57899067393956	C
-4.86647443745153	3.22088616342794	3.27495371489260	C
-2.29613769778981	3.11003622466772	3.76043419065882	C
1.31555796236836	0.59575723537650	3.58756333675309	C

2.36853208414282	3.03879757030189	3.77570006662610	C
4.94429355622768	3.07090935632327	3.30725394323850	C
0.07051683175184	5.40053160803552	4.13201823321497	S
-10.02764842724427	-10.13982754000178	1.24748075257192	H
9.70496151730980	-10.44146499118176	1.30158989411805	H
-9.52072343369057	2.55052074423618	0.35497883198051	C
9.59243467769110	2.25859791445428	0.41320219003050	C
-13.67622943483868	-1.57132012411162	0.90094942224433	H
-13.72997950405668	-6.58277163143874	0.88473857753792	H
13.61641854121187	-1.98905512365326	0.97889806823494	H
13.51651869018055	-6.99989725129758	0.96327388356885	H
5.95898950584250	-13.69058221608991	1.67561216527818	H
-6.38462635240351	-13.50183640240216	1.64277227549828	H
-5.97958353629888	4.92249523407296	3.29641637070320	H
6.10903612739573	4.73765979774568	3.33654645973484	H
8.14250513109799	3.96434724515314	-0.73788558921218	N
-8.01310432720719	4.21086536540783	-0.78808280113116	N
9.71129918008110	5.66400287766390	-1.88055571325538	C
-9.52264950931372	5.95890855789478	-1.93728656242079	C
-12.17760699479305	3.23258617863897	-0.04992864077168	C
-12.16628756897257	5.37681630181080	-1.45048742063599	C
12.27112226710546	2.85822836103780	0.02184635384369	C
12.33317162961162	5.00103792112889	-1.37965183836696	C
-13.81115865945752	2.29982738818281	0.72207792904103	H
-13.77576024805034	6.45673903157062	-2.08337137034200	H
13.97848614557018	6.03023066006471	-2.00501094500941	H
13.87111955835950	1.87620685845253	0.80309123985056	H
8.71872278033867	7.62991392949797	-3.28932053630873	C
-8.46230432650254	7.89447500878998	-3.33863792206030	C
6.11762146622260	8.09123296776899	-3.65466059938634	C
-5.84624969809195	8.27555595539953	-3.68909817463217	C
3.71347626147013	6.17310913600684	-2.37216013090437	S
-3.50981522402199	6.28384463756604	-2.39397075114971	S
1.44870867508904	8.11666047018064	-3.67961137759403	C
5.12767923254872	10.13225117003430	-5.04449462215482	C
2.50428332703314	10.15156772854778	-5.05932692581410	C
-1.17870929846554	8.15710419367236	-3.68727340456453	C
-2.16313372648914	10.22368373607066	-5.07249436316767	C
-4.78591772491255	10.28532094938991	-5.07252502885347	C
0.20430570991038	12.12978900367945	-6.38202632994929	S
-5.93660803742551	11.69592342825213	-5.99874832647616	H
6.32661643784052	11.50663352617899	-5.96400955120214	H
-9.71071413440391	9.24851125091526	-4.23648283741096	H
10.01323892873320	8.94402228580086	-4.18132078516325	H

Singlet state of molecule 1b, B3LYP

The atomic coordinates in atomic units optimized at the B3LYP/def2-TZVP level.

2.87508906457794	0.00000000000000	-8.23995721950260	C
-2.87508906457794	0.00000000000000	-8.23995721950260	C
1.33125158347559	0.00000000000000	-6.06567320203940	C
-1.33125158347559	0.00000000000000	-6.06567320203940	C
-3.21804874211097	0.00000000000000	-3.34916921762667	S
3.21804874211097	0.00000000000000	-3.34916921762667	S
6.01402523741714	0.00000000000000	-5.11834747857948	C
5.41574145427645	0.00000000000000	-7.72055627634694	C
-6.01402523741714	0.00000000000000	-5.11834747857948	C
-5.41574145427645	0.00000000000000	-7.72055627634694	C
-8.47280796129317	0.00000000000000	-4.17688617596460	C
-9.32477095285662	0.00000000000000	-1.67990507733064	C
8.47280796129317	0.00000000000000	-4.17688617596460	C

9.32477095285662	0.00000000000000	-1.67990507733064	C
7.82271044225370	0.00000000000000	0.38355508989914	N
-7.82271044225370	0.00000000000000	0.38355508989914	N
9.37777001659978	0.00000000000000	2.41441402543901	C
12.01213853011365	0.00000000000000	1.61960661754316	C
11.98077533283013	0.00000000000000	-0.93927220368636	C
-9.37777001659978	0.00000000000000	2.41441402543901	C
-12.01213853011365	0.00000000000000	1.61960661754316	C
-11.98077533283013	0.00000000000000	-0.93927220368636	C
8.49637047663384	0.00000000000000	4.90562395418378	C
5.96180998590381	0.00000000000000	5.60415558329825	C
-8.49637047663384	0.00000000000000	4.90562395418378	C
-5.96180998590381	0.00000000000000	5.60415558329825	C
3.53953376017526	0.00000000000000	3.32237518927477	S
-3.53953376017526	0.00000000000000	3.32237518927477	S
1.30033030237051	0.00000000000000	5.67698822738207	C
4.97298720470144	0.00000000000000	8.09682561845789	C
2.36377709664540	0.00000000000000	8.13098177854972	C
-1.30033030237051	0.00000000000000	5.67698822738207	C
-2.36377709664540	0.00000000000000	8.13098177854972	C
-4.97298720470144	0.00000000000000	8.09682561845789	C
9.93194339162102	0.00000000000000	-5.61811699650026	H
-9.93194339162102	0.00000000000000	-5.61811699650026	H
9.88334301805738	0.00000000000000	6.41380379710610	H
-9.88334301805738	0.00000000000000	6.41380379710610	H
13.63339642990538	0.00000000000000	2.85830711299194	H
13.57252307525767	0.00000000000000	-2.21604723769783	H
-13.63339642990538	0.00000000000000	2.85830711299194	H
-13.57252307525767	0.00000000000000	-2.21604723769783	H
-6.87786682417240	0.00000000000000	-9.14907044501871	H
6.87786682417240	0.00000000000000	-9.14907044501871	H
6.18784230616849	0.00000000000000	9.73893758401449	H
-6.18784230616849	0.00000000000000	9.73893758401449	H
-2.11316953721287	0.00000000000000	-10.13317286520490	H
2.11316953721287	0.00000000000000	-10.13317286520490	H
0.00000000000000	0.00000000000000	10.47947469865923	S

Triplet state of molecule 1b^{2+}, B3LYP

The atomic coordinates in atomic units optimized at the B3LYP/def2-TZVP level.

-2.82960452609225	-8.61610516034017	-0.12282639654050	C
2.87739657230757	-8.60057586060839	-0.10387513728182	C
-1.31159644884760	-6.41033278170002	-0.08732019484907	C
1.34719844975058	-6.40310753348957	-0.07793209610004	C
3.19250194564608	-3.67130335889536	-0.03324339535118	S
-3.17199651249477	-3.68858783679956	-0.05674531395072	S
-5.93342235801328	-5.48385501199007	-0.09172587286547	C
-5.36111733063574	-8.10299854651426	-0.12489755196392	C
5.96383539169670	-5.45149459176169	-0.05030249634881	C
5.40603616975412	-8.07369049115823	-0.08899558929047	C
8.42084361847599	-4.51522338788783	-0.03027962446265	C
9.22359450552027	-2.00241031350555	0.00680436812711	C
-8.39558062089252	-4.56098700797816	-0.08944144150745	C
-9.21229513558626	-2.05256536243050	-0.06079147464912	C
-7.66221001761727	-0.02080689493659	-0.02892446580718	N
7.66220540414557	0.02079198773571	0.03006712396461	N
-9.22357912807859	2.00246331290264	-0.01086644294788	C
-11.88916503661812	1.23783291635937	-0.03237428678678	C
-11.88210162295661	-1.30247675773343	-0.06320132925182	C
9.21228624147389	2.05253198900039	0.06331091167681	C
11.88210762195645	1.30249369071163	0.06184549133331	C

11.88919062635235	-1.23774623930408	0.02570450701765	C
-8.42082222724571	4.51529795876145	0.02458126571646	C
-5.96382681977376	5.45152475631931	0.04793807109170	C
8.39556266609465	4.56092152313444	0.09442481498238	C
5.93340091555178	5.48377914518162	0.09752524240415	C
-3.19251374148581	3.67125456600518	0.03684788623335	S
3.17197730053825	3.68852025876948	0.06192262518136	S
-1.34720871708122	6.40307216796914	0.08064345156315	C
-5.40602318852564	8.07374279866869	0.08503167029661	C
-2.87739420411683	8.60059146826796	0.10272246807400	C
1.31157949883562	6.41027408028103	0.09186079525885	C
2.82958533701704	8.61603836280119	0.12797805276500	C
5.36109596719799	8.10292229634409	0.13073288731916	C
-9.86356239962857	-5.99092118097620	-0.11451752170580	H
9.89675906121263	-5.93710223088869	-0.04599295169831	H
-9.89672127973295	5.93723512043647	0.03590942650626	H
9.86354652030445	5.99086067927129	0.11911625045717	H
-13.48614175535725	2.50521980875801	-0.02406972048663	H
-13.47200655147593	-2.57855129132507	-0.08593369311860	H
13.47201054935948	2.57855893227419	0.08525160629999	H
13.48618521560553	-2.50507012083428	0.01257988113515	H
6.88198077769994	-9.48632560574117	-0.10507721151737	H
-6.82921255367840	-9.52367201663897	-0.14928869545758	H
-6.88195663761674	9.48642431937166	0.09767176000710	H
6.82919110359207	9.52359243670135	0.15534728457233	H
2.05919152114926	10.50375331305044	0.15065749398855	H
-2.11745635845922	10.49247396815441	0.13015021037622	H
2.11746265606997	-10.49244323352048	-0.13243098262054	H
-2.05921046529738	-10.50381904027299	-0.14557165978851	H

Singlet state of molecule $\mathbf{1b^{2+}}$, B3LYP

The atomic coordinates in atomic units optimized at the B3LYP/def2-TZVP level.

2.88766857291685	0.00000000000000	-8.27240932057557	C
-2.88766857291685	0.00000000000000	-8.27240932057557	C
1.36724441864565	0.00000000000000	-6.11296875560116	C
-1.36724441864565	0.00000000000000	-6.11296875560116	C
-3.17498535680249	0.00000000000000	-3.38848452050362	S
3.17498535680249	0.00000000000000	-3.38848452050362	S
5.98385788623435	0.00000000000000	-5.11812082823547	C
5.44544539716308	0.00000000000000	-7.71853042835273	C
-5.98385788623435	0.00000000000000	-5.11812082823547	C
-5.44544539716308	0.00000000000000	-7.71853042835273	C
-8.44989846676871	0.00000000000000	-4.15485222426470	C
-9.33698522661767	0.00000000000000	-1.66427579050698	C
8.44989846676871	0.00000000000000	-4.15485222426470	C
9.33698522661767	0.00000000000000	-1.66427579050698	C
7.81598359068157	0.00000000000000	0.38974877865935	N
-7.81598359068157	0.00000000000000	0.38974877865935	N
9.38753608766317	0.00000000000000	2.40771269103782	C
12.02000826048506	0.00000000000000	1.62585280492873	C
11.98971740912054	0.00000000000000	-0.93312693376039	C
-9.38753608766317	0.00000000000000	2.40771269103782	C
-12.02000826048506	0.00000000000000	1.62585280492873	C
-11.98971740912054	0.00000000000000	-0.93312693376039	C
8.46865078573306	0.00000000000000	4.89729846672367	C
5.92526939011177	0.00000000000000	5.60152948116066	C
-8.46865078573306	0.00000000000000	4.89729846672367	C
-5.92526939011177	0.00000000000000	5.60152948116066	C
3.50366430670936	0.00000000000000	3.33788597580190	S
-3.50366430670936	0.00000000000000	3.33788597580190	S

1.31667645802170	0.00000000000000	5.70063270597750	C
4.97961573265174	0.00000000000000	8.09937276121278	C
2.34530631445187	0.00000000000000	8.15495297439999	C
-1.31667645802170	0.00000000000000	5.70063270597750	C
-2.34530631445187	0.00000000000000	8.15495297439999	C
-4.97961573265174	0.00000000000000	8.09937276121278	C
9.90507291682642	0.00000000000000	-5.60228005406380	H
-9.90507291682642	0.00000000000000	-5.60228005406380	H
9.84910443765635	0.00000000000000	6.41415195367264	H
-9.84910443765635	0.00000000000000	6.41415195367264	H
13.63986032061860	0.00000000000000	2.86385091878855	H
13.58182154425434	0.00000000000000	-2.20696167925282	H
-13.63986032061860	0.00000000000000	2.86385091878855	H
-13.58182154425434	0.00000000000000	-2.20696167925282	H
-6.92120653631610	0.00000000000000	-9.13268874473923	H
6.92120653631610	0.00000000000000	-9.13268874473923	H
6.20825335354335	0.00000000000000	9.73244974865402	H
-6.20825335354335	0.00000000000000	9.73244974865402	H
-2.14945327727273	0.00000000000000	-10.17375047476519	H
2.14945327727273	0.00000000000000	-10.17375047476519	H
0.00000000000000	0.00000000000000	10.50602098720786	S

Singlet state of molecule 2b, B3LYP

The atomic coordinates in atomic units optimized at the B3LYP/def2-TZVP level.

-0.00652726866594	-10.17324794229102	0.16684312351841	S
-2.37845479054436	-7.82404239693610	0.11262819986297	C
2.36840316079801	-7.82670963050388	0.13419670858391	C
-1.30542588098389	-5.37436661905771	0.06986183002874	C
1.29858918936569	-5.37587292994343	0.08157088494495	C
3.53673913989511	-3.03026148983127	0.05119911756549	S
-3.54053585603962	-3.02604325279296	0.02038528187721	S
-5.97782486729947	-5.28159653539622	0.05776720391505	C
-4.99348629987681	-7.77971558752288	0.10507962984844	C
5.97094053184010	-5.28844145830996	0.11016292798614	C
4.98336042915584	-7.78531666540997	0.15038066299567	C
8.50184508022013	-4.55538461054013	0.11538131807078	C
9.39464056783789	-2.06221052113557	0.07712670512313	C
-8.50799877961052	-4.54560402759008	0.04252911212226	C
-9.39749617121803	-2.05118240868964	0.00066216111288	C
-7.87468347673967	0.00464563602754	-0.03089234088966	N
7.87470637957273	-0.00464162638151	0.03039040742969	N
-9.39478556494793	2.06238450075485	-0.06719765537365	C
-12.03776180239147	1.28847050171304	-0.05869031911883	C
-12.03944913543211	-1.27391946189010	-0.01585321072517	C
9.39738233452690	2.05123637586717	0.00336591003689	C
12.03927208827696	1.27417768441376	0.03391454698336	C
12.03755662851637	-1.28805884547916	0.08081452266926	C
-8.50201264122754	4.55569430662909	-0.10628026492489	C
-5.97089534935510	5.28854542437657	-0.11020550811931	C
8.50790115572385	4.54541456131161	-0.04592720415027	C
5.97793298753062	5.28131092405682	-0.06902739318345	C
-3.53660675692980	3.03004792172371	-0.05782180000275	S
3.54068857847519	3.02591996990624	-0.03348794943196	S
-1.29839441999996	5.37566641824847	-0.09364145557312	C
-4.98324933287283	7.78544981297275	-0.15322043674930	C
-2.36817858729951	7.82660915912601	-0.14470775446441	C
1.30562374932475	5.37410304581383	-0.08495792928435	C
2.37870912682189	7.82368732935251	-0.12899276943254	C
4.99364339313265	7.77929760416365	-0.12009270840087	C
0.00687718287397	10.17297944827072	-0.18240913893331	S

-9.90693773693899	-6.04293423116772	0.06659886145213	H
9.89862496295832	-6.05418650975193	0.15323854582484	H
-9.89898514778734	6.05475056952919	-0.13636147893993	H
9.90672025177427	6.04263097119355	-0.06783618051778	H
-13.64506311867889	2.54507883843392	-0.08178662475600	H
-13.64839964612512	-2.52848933277018	0.00276761334821	H
13.64813541693194	2.52874788122255	0.02142496733023	H
13.64473611501029	-2.54439771336825	0.11447636626363	H
6.19816871295366	-9.42645971183702	0.19008801333309	H
-6.21055855824008	-9.41958586960643	0.13285512548414	H
-6.19815892213215	9.42678514460401	-0.18825219376217	H
6.21067294782016	9.41903534849152	-0.14806743097788	H

Triplet state of molecule $2b^{2+}$, B3LYP

The atomic coordinates in atomic units optimized at the B3LYP/def2-TZVP level.

-0.00670204950439	-10.19809518786959	0.17230216440873	S
-2.36141845524045	-7.84324693831162	0.12305257742673	C
2.35111607855986	-7.84603297202582	0.14218521842107	C
-1.30160904725603	-5.37194479652005	0.08663550907745	C
1.29455026966537	-5.37347638787410	0.09707682121181	C
3.51139055951720	-3.01729422914092	0.06604029261330	S
-3.51535084939104	-3.01314681749737	0.03765482808131	S
-5.93599649704629	-5.26439820273751	0.06411810907333	C
-4.97440034769980	-7.78588048672075	0.11068558245174	C
5.92909855091472	-5.27140997488274	0.11153941440667	C
4.96417224149325	-7.79174969782862	0.15093318925397	C
8.46986649684247	-4.55110253807521	0.10930386511491	C
9.37069949676273	-2.05206376540441	0.07005123745869	C
-8.47582853210828	-4.54107447131943	0.04253897847880	C
-9.37337660665494	-2.04097573962215	-0.00337892578875	C
-7.83961360825031	0.00439747090424	-0.04077629505272	N
7.83969205860316	-0.00487449592187	0.02110856906266	N
-9.37060716494339	2.05199776075733	-0.07019075415159	C
-12.03450228045551	1.28116388943926	-0.05176235288567	C
-12.03622768820269	-1.26636331389281	-0.01078699991569	C
9.37328675773044	2.04090830111041	0.00341790327205	C
12.03605061907601	1.26691931760606	0.04196608471119	C
12.03445998052189	-1.28063096778372	0.08150530364999	C
-8.46973172050272	4.55100265804016	-0.10908758433906	C
-5.92897089687948	5.27110335635593	-0.13114385244058	C
8.47568439902077	4.54099690440073	-0.04154525362187	C
5.93602654089171	5.26410710924154	-0.08261138493840	C
-3.51121766512575	3.01658745400073	-0.13177645982755	S
3.51568582269814	3.01244290045455	-0.10268630972843	S
-1.29436863343762	5.37296311512820	-0.14589117541591	C
-4.96413025277725	7.79170407879610	-0.14798383819000	C
-2.35105600889516	7.84587596754320	-0.15306890676376	C
1.30181390680319	5.37142857493295	-0.13501733810132	C
2.36143593016582	7.84310632322408	-0.13328280322186	C
4.97430458766473	7.78585388062562	-0.10626194109893	C
0.00661505859813	10.19826337707878	-0.15274042736794	S
-9.87154915040895	-6.04064423637706	0.06616775868587	H
9.86359651140548	-6.05233232755007	0.14293196463153	H
-9.86344801931691	6.05259912529031	-0.11874064199540	H
9.87122465473482	6.04092847989199	-0.04114969964332	H
-13.63586731432317	2.54295264077741	-0.06939009110660	H
-13.63929273090270	-2.52584919611532	0.01489913282555	H
13.63898382971979	2.52683061346800	0.03796198296021	H
13.63581707865017	-2.54205806453814	0.11670901152001	H
6.19396214211275	-9.42248915312044	0.18312092693898	H

```
-6.20633026140248     -9.41517425797544      0.13247446310305  H
-6.19395639341565      9.42273758867440     -0.15005486117780  H
 6.20601860198848      9.41543733136306     -0.09705299206643  H
```

Signed modulus plots of the current density

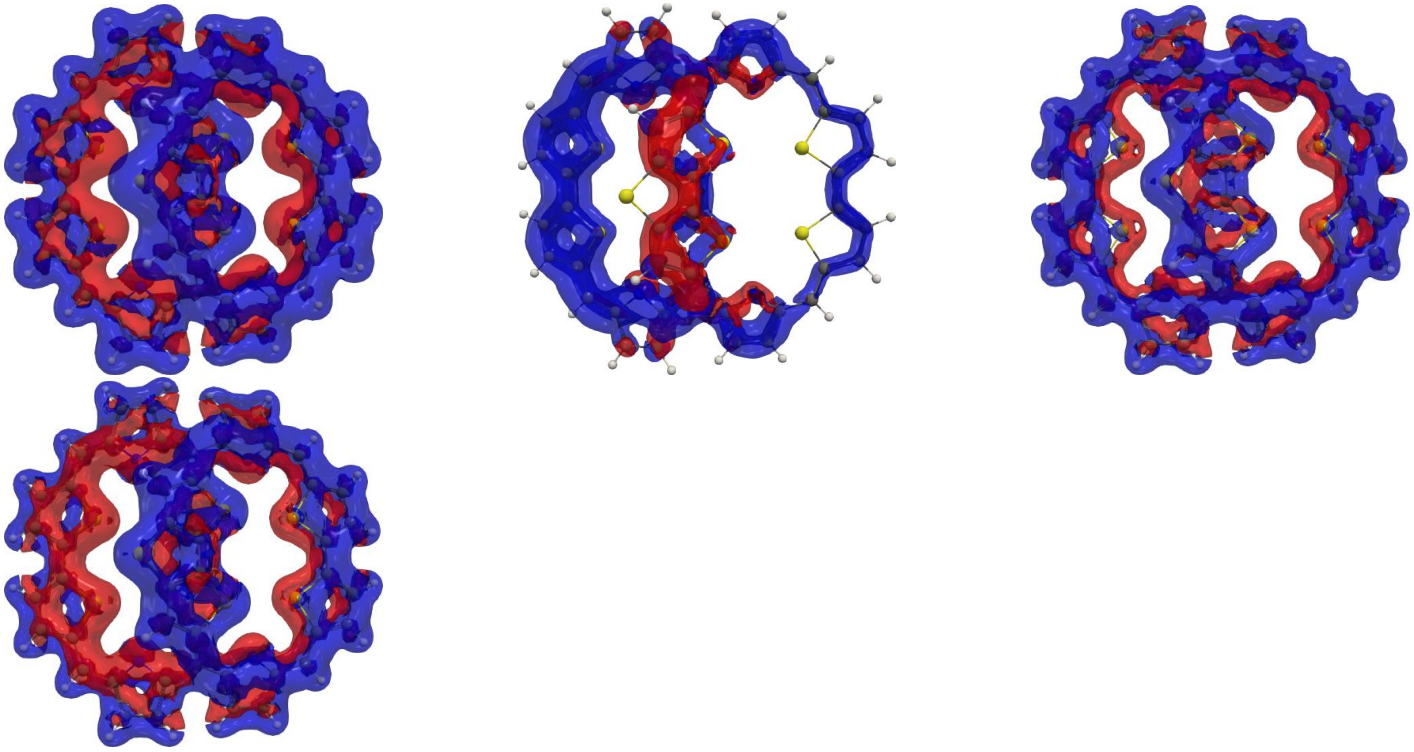


Fig. 4 Calculated a) signed modulus of the total current density, b) the (α - β) spin current density and c) the α contribution and d) β contribution to the total current density of **1a**$^{2+}$. For all isosurfaces an isovalue of 0.02 has been used.

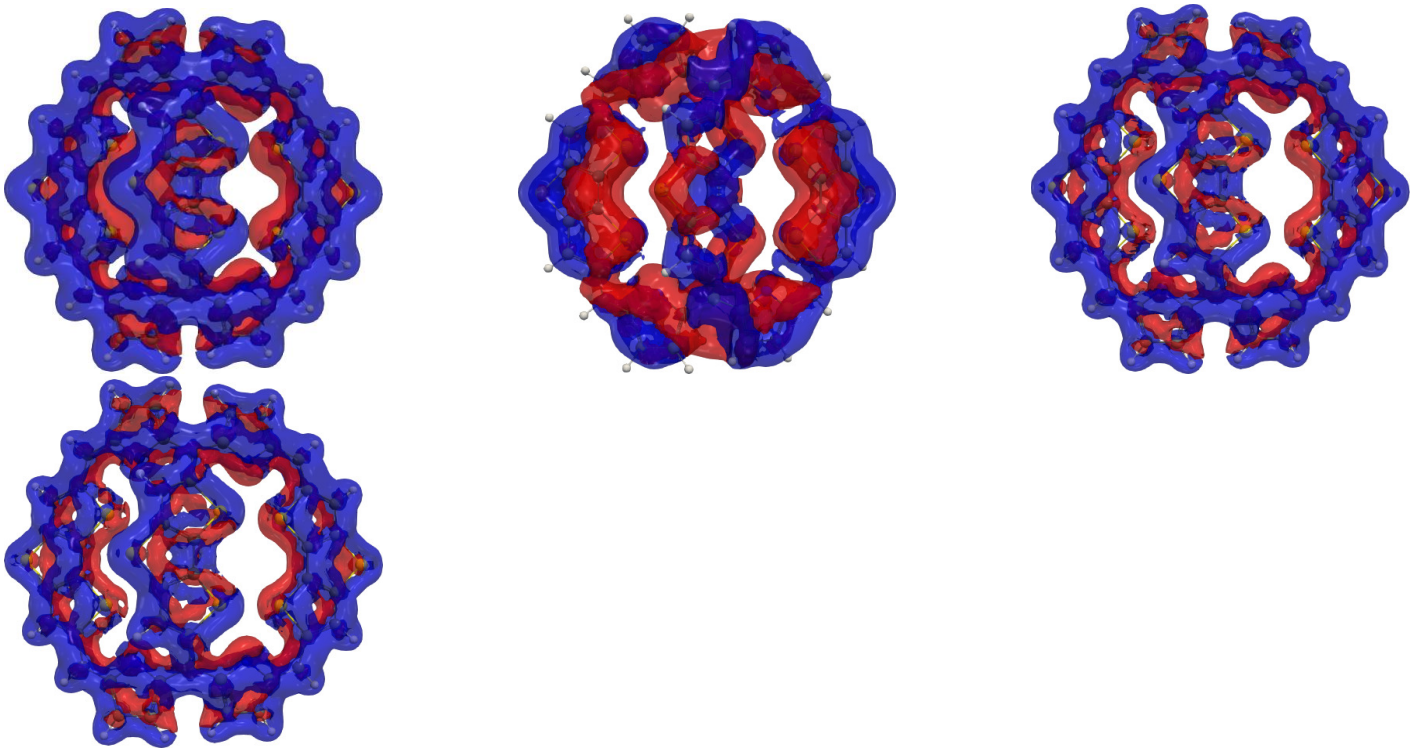


Fig. 5 Calculated a) signed modulus of the total current density, b) the (α - β) spin current density and c) the α contribution and d) β contribution to the total current density of **2a**$^{2+}$. For isosurfaces a), c) and d) an isovalue of 0.02 has been used, while for b) an isovalue of 0.002 has been adopted.

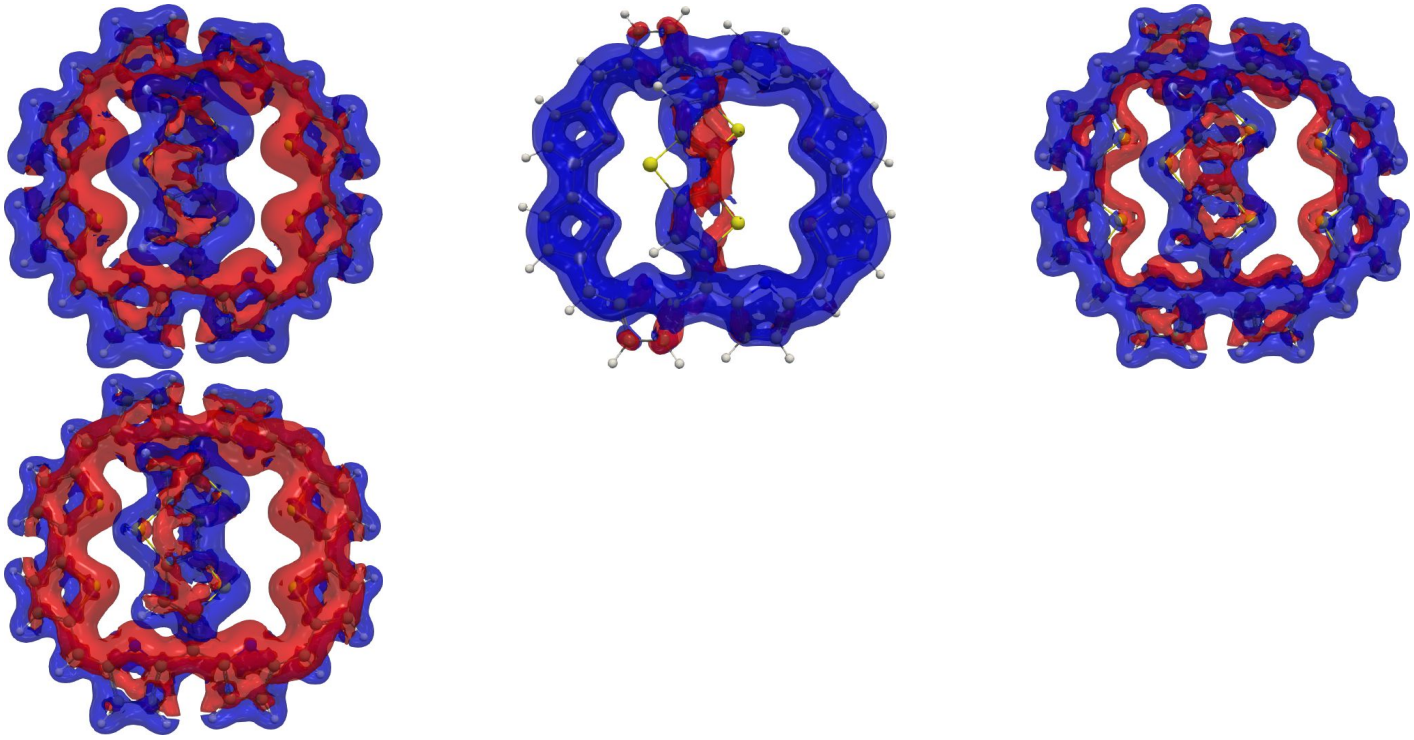


Fig. 6 Calculated a) signed modulus of the total current density, b) the (α - β) spin current density and c) the α contribution and d) β contribution to the total current density of **1a**$^{+}$. For all isosurfaces an isovalue of 0.02 has been used.

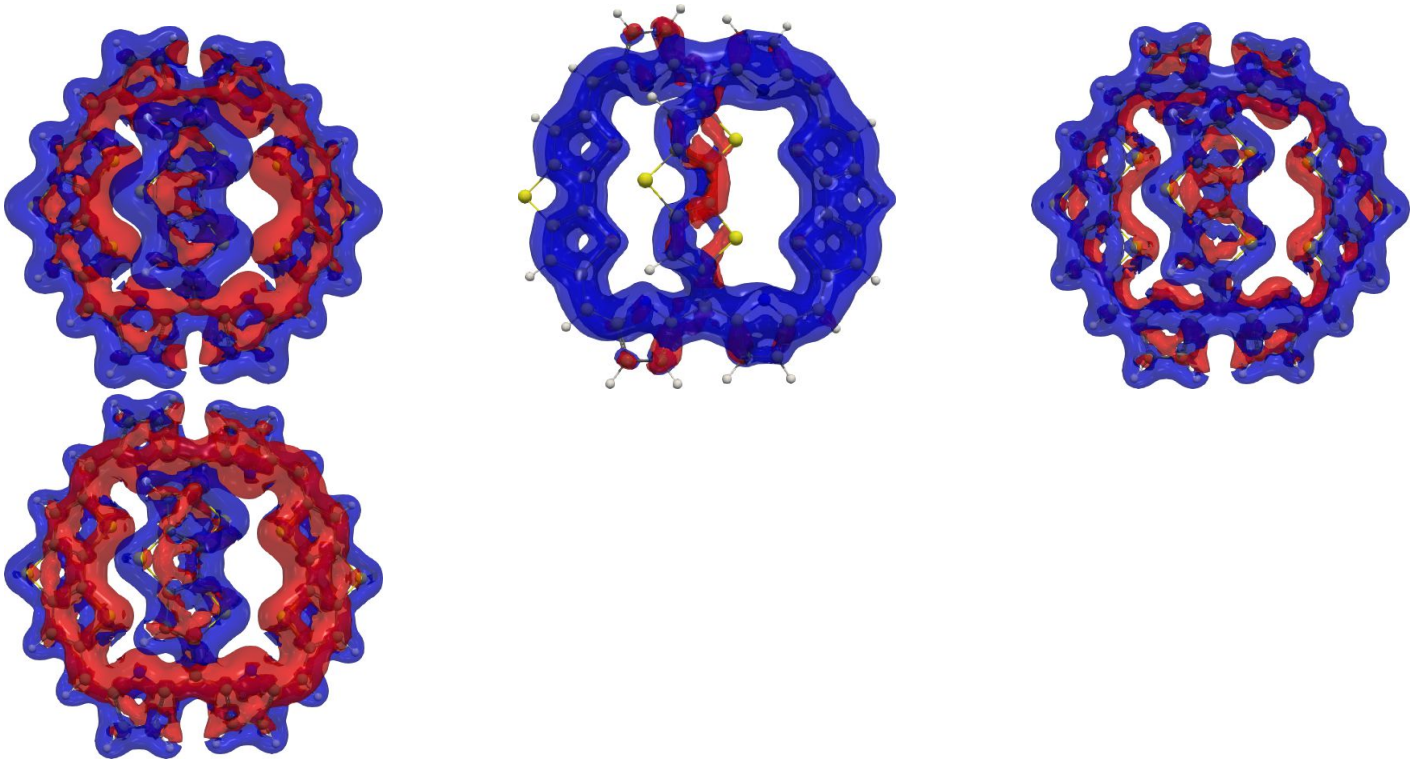


Fig. 7 Calculated a) signed modulus of the total current density, b) the (α - β) spin current density and c) the α contribution and d) β contribution to the total current density of **2a**$^{+}$. For all isosurfaces an isovalue of 0.02 has been used.