Supporting Information

Dissecting the Single-Electron C–C Bond: NBO and AIM Perspectives

Leonardo I. Lugo-Fuentes,[a] Darien I. Martínez-Valencia,[a] J. Oscar C. Jiménez-Halla,[a] and Joaquín Barroso-Flores[b,c]*

[a]*Department of Chemistry, Division of Natural and Exact Sciences, University of Guanajuato, Campus Gto, Noria Alta s/n, 36050 Guanajuato, Mexico.*
[b]*Centro Conjunto de Investigación en Química Sustentable UAEM-UNAM, Unidad San Cayetano, 50200 Toluca de lerdo, México.*
[c]*Instituto de Química, Universidad Nacional Autónoma de México, Circuito Exterior S/N, Ciudad Universitaria, alcaldía de Coyoacán, CP 04510, Ciudad de México, México.*

Table of Contents

Non-Covalent Interactions (NCI)

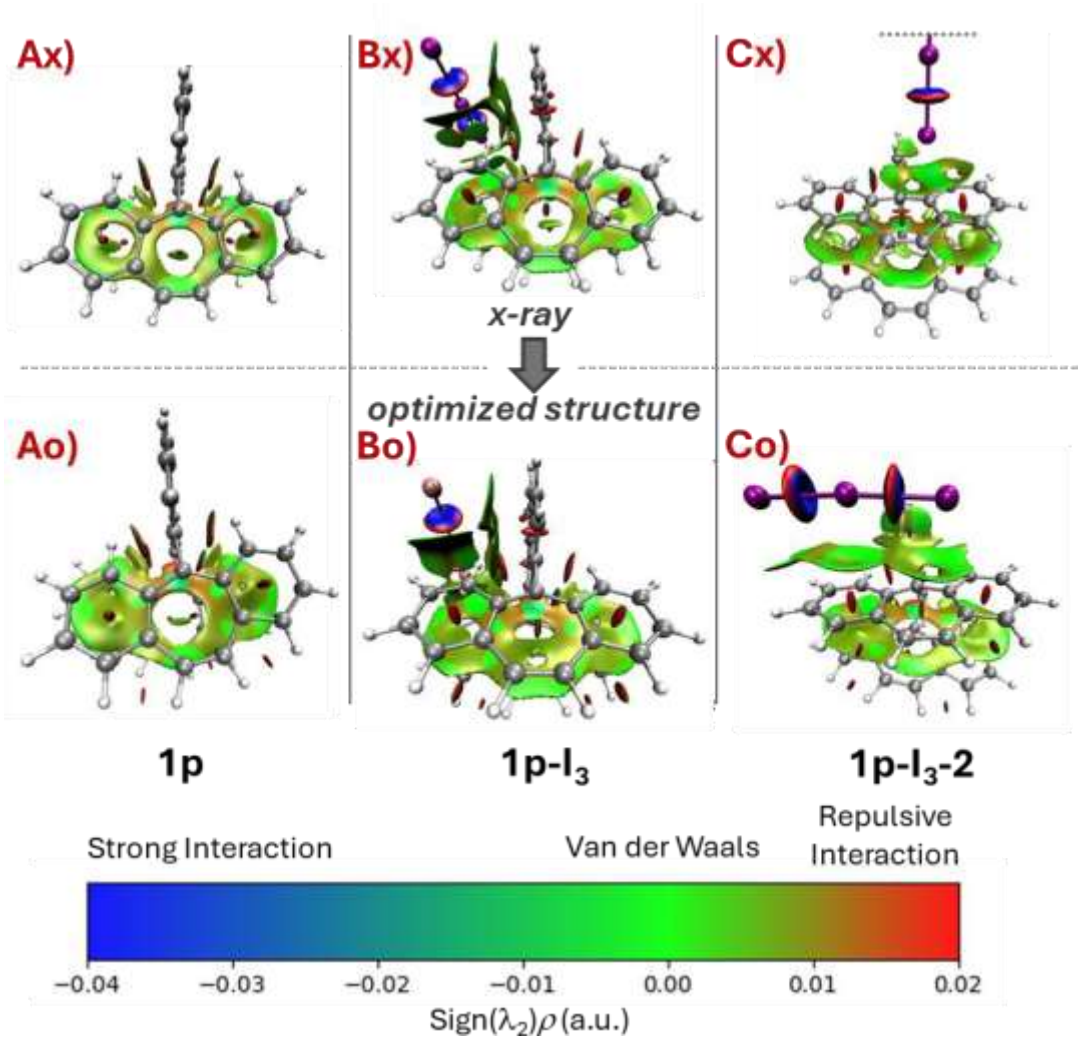


Figure S1. Non-Covalent Interaction (NCI) iso-surfaces of the different chosen X-ray structures and the optimized structures of **1p**.

Atoms In Molecules (AIM)

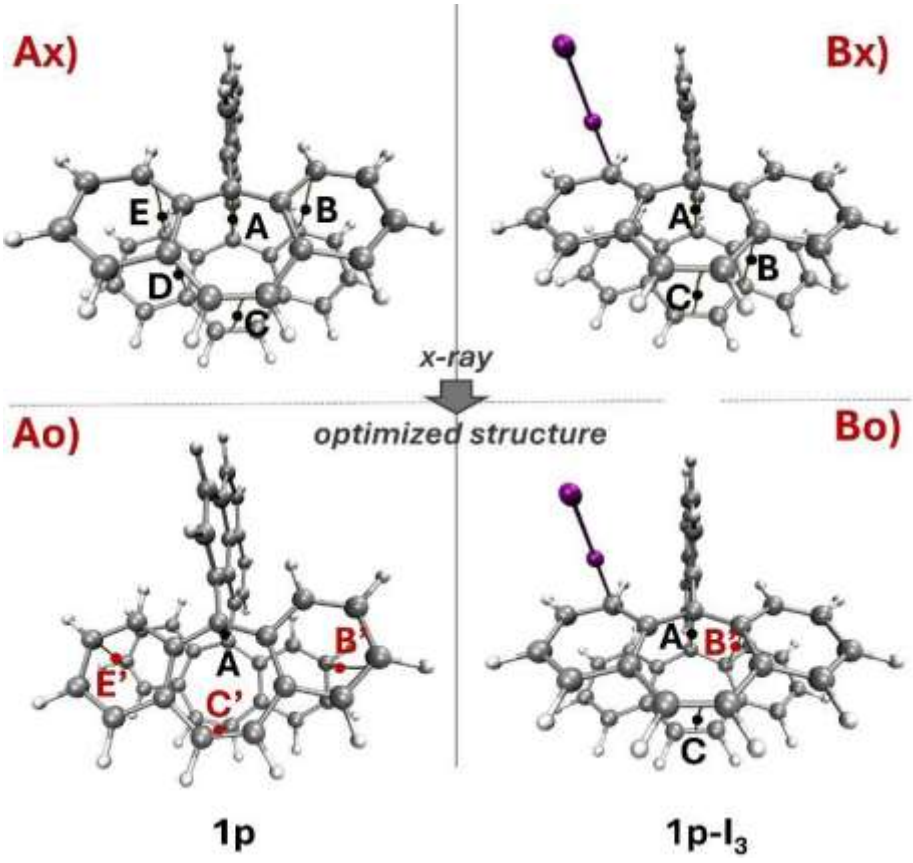


Figure S2. Bond Critical Points (BCPs) for different X-ray and optimized structures of **1p**. Red labels in the BCP correspond to those that changed with respect to the X-ray structure. Only relevant bond paths and BCP are shown between the tricyclic structures

Table S1. Comparison between Multiwfn and DTK of the Bond Critical Points (BCP) for the following X-ray structures showing the electron density, $\rho(r)$, Laplacian density, $\nabla^2\rho(r)$, shown in atomic units.

				Multiwfn		**DensToolKit2 (DTK)**	
Entry	**Structure**	**BCP**	**atoms**	**$\rho(r)$**	**$\nabla^2\rho(r)$**	**$\rho(r)$**	**$\nabla^2\rho(r)$**
1	**1**			0.147	-0.141	0.147	-0.141
2	**1p-I_3**	A	C1-C2	0.013	0.029	0.013	0.029
3	**1pp-I_3**			0.009	0.029	0.009	0.029
4	**1p-B**	A'	B1-B2	0.040	-0.001	0.040	-0.001

Natural Bond Critical Point

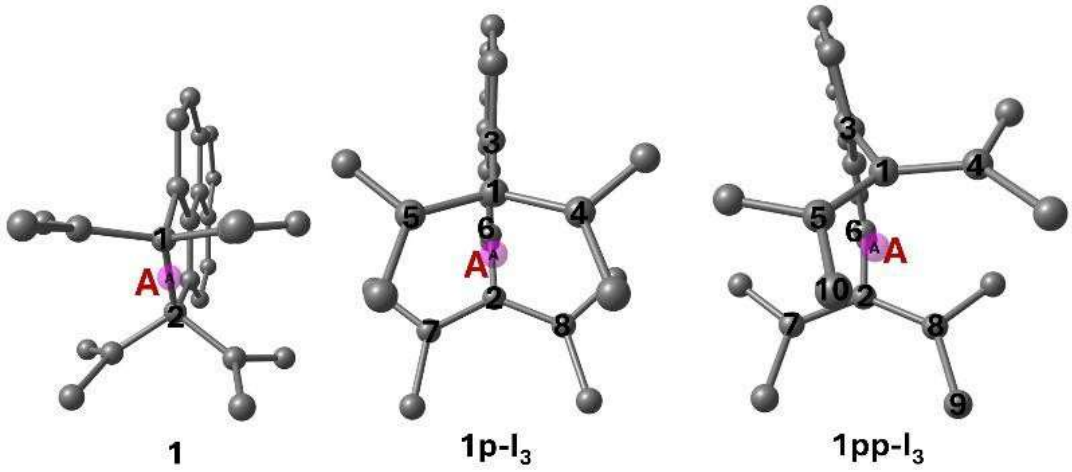
Herein, we examine the topological features of the previously calculated BCP **A** from a distinct perspective using Natural Bond Critical Point (NBCP) theory, using NBO 7.0 version. Like AIM, NBCP theory determines bond critical points based on total electron density but expresses this density in terms of Natural Atomic Orbitals (NAOs) or Natural Bond Orbitals (NBOs). This approach enables the identification of the specific NBOs that contribute most significantly to a given BCP. Applying this method to the optimized structures of **1**, **1p-I_3** and **1pp-I_3** reveals the following insights (**Table S2**): for molecule **1**, the electron density ($\rho(r)$ = 0.1597 a.u.) and the Laplacian of the electron density ($\nabla^2\rho(r)$ = −0.1084 a.u.) at BCP **A** fall within the range expected for a typical covalent bond. In this case, a single NBO, σ(C1-C2), accounts for 100% of the electron density at BCP **A**. Moreover, the difference in electron density between AIM and NBCP analysis is minimal (0.0007 e^-), indicating good agreement between both methods.

In contrast, for the cationic and dicationic structures, the BCP **A** is composed of multiple NBO contributions, none exceeding 30%. This suggests that no single NBO dominates the electron density at this critical point. For the cationic structure **1p-I_3**, NBCP analysis separates the contributions of α and β electrons at BCP **A**, revealing two main differences: 1) The α-electron density (0.0082 e^-) is more than twice that of the β-electron density (0.0029 e^-); and 2) the primary NBOs contributing to the α-electron density are π(C1-C4) (22.9%) and π(C2-C8) (22.2%), followed by their corresponding antibonding orbitals π^*(C1-C4) (4.4%) and π^*(C2-C8) (4.7%). In the β channel, the leading contributors are the low-valence orbitals (LV) with occupancies below 0.5e^-, LV(C1) (27.7%) and LV(C2) (26.6%) followed by σ(C2-C6) (7.1%) and σ(C1-C3) (4.3%). In both spin channels, these NBOs do not account for the full electron density, as additional contributions from non-occupied orbitals amount to 38.8% (α) and 24.9% (β), as shown in **Table S2**. Thus, NBCP analysis confirm that in **1p-I_3**, the electron density at BCP **A** results from a combination of several NBOs, rather than a single dominant orbital.

For the dicationic structure, **1pp-I_3**, NBCP analysis shows that BCP **A** between C1 and C2 persists, but the electron density at this point decreases from $\rho(r)$ = 0.0111 e^- in **1p-I_3** to $\rho(r)$ = 0.0050 e^-. The main contributors are two three-center two-electron bonds (3C): 3C(C2-C8-C9) (25.4%) and 3C(C1-C5-C10) (24.5%), along with their non-Lewis counterparts, $3C_n$(C2-C8-C9) (8.5%) and $3C_n$(C1-C5-C10) (9.3%). Again, these orbitals do not fully account for the electron density, indicating that multiple NBOs contribute to the interaction between the ipso carbons.

In summary, NBCP analysis suggests that in **1p-I_3**, the interaction between C1 and C2 arises from a broad mix of Lewis-type NBOs, σ(C-C) and π(C-C) bonds, and non-Lewis-type orbitals. Given the presence of both types, the interaction can be further characterized either by estimating the second-order perturbation energy, E(2), for donor-acceptor interactions or by using NBO deletion analysis to directly calculate the interaction energy from the Fock matrix. In the next section, we applied the latter method to explore these interactions in more detail.

Table S2. NBCP analysis of the neutral, **1**, cationic, **1p-I$_3$**, and dicationic, **1pp-I$_3$** optimized structures, showing the electron density, $\rho(r)$, Laplacian density, $\nabla^2\rho(r)$, values of the NBCP **A**. The QTAIM and NBCP density difference at BCP **A** is given as $\rho(r)_{BCP}$ - $\rho(r)_{NBCP}$, with the corresponding NBOs and the contribution percentage to the electron density. For clarity, only relevant atoms of each analyzed structure are shown.

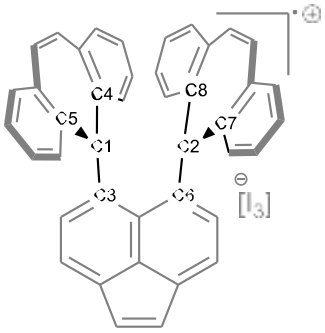


	NBCP	$\rho(r)^a$	$\nabla^2\rho(r)^a$	$\rho(r)_{BCP}$– $\rho(r)_{NBCP}$	NBO	%ρ
1	**A**	0.1597	-0.1084	0.0007	σ(C1-C2)	100%
1p-I$_3$	**A** (alpha)	0.0082	0.0139	0.0016	σ(C2-C6)	
					σ(C2-C8)	2.8%
					π(C1-C4)	1.4%
					σ(C1-C3)	22.9%
					π(C2-C8)	1.2%
					π*(C1-C4)	22.2%
					π*(C2-C8)	4.4%
					σ(C2-C6)	4.7%
					others	2.8%
	A (beta)	0.0029	0.0121	0.0015	σ(C2-C6)	7.1%
					π(C1-C4)	3.6%
					σ(C1-C3)	4.3%
					σ(C1-C5)	3.3%
					π(C2-C8)	2.4%
					LV(C1)	27.7%
					LV(C2)	26.6%
					others	24.9%

					σ(C2-C6)	
					σ(C2-C8)	
					σ(C1-C3)	
					σ(C1-C5)	2.9%
					3C	5.0%
					(C2-C8-	2.5%
					C9)	4.5%
					3C	
					(C1-C5-	25.4%
					C10)	
					$3C_n$	24.5%
1pp-I_3	**A**	0.0050	0.0206	0.0039	(C2-C8-	
					C9)	8.5%
					$3C_n$	
					(C1-C5-	9.3%
					C10)	
					3C*	1.8%
					(C2-C8-	
					C9)	1.3%
					3C*	14.4%
					(C1-C5-	
					C10)	
					others	

[a]Calculated according to the NBCP theory.

Table S3. Natural Bond Orbital Deletion energies (kcal/mol) of the interacting donor-acceptor orbitals of C1 and C2. Two types of acceptor orbitals are shown: antibonding **σ*/π*** and Rydberg *p*-orbitals of C1 and C2 **Ry [p(C)]** (see **Figure 10** of the manuscript).



Entry	Donor orbital	Acceptor orbital	Type σ*/π*	Deletion energy	Acceptor orbital (Ridberg)	Type Ry[p(C)]	Deletion energy
1A	σ(C2-C6)	1A*, 2A*, 3A* 4A*	σ*(C-C) π*(C-C)	0.036	$1A^{Ry}$, $2A^{Ry}$, $3A^{Ry}$	*p*(C)	0.181
2A	σ(C2-C8)	1A*, 2A*, 3A* 4A*	σ*(C-C) π*(C-C)	0.008	$1A^{Ry}$, $2A^{Ry}$, $3A^{Ry}$	*p*(C)	0.229
3A	σ(C2-C7)	1A*, 2A*, 3A* 4A*	σ*(C-C) π*(C-C)	0.032	$1A^{Ry}$, $2A^{Ry}$, $3A^{Ry}$	*p*(C)	0.248
4A	π(C2-C7)	1A*, 2A*, 3A* 4A*	σ*(C-C) π*(C-C)	0.179	$1A^{Ry}$, $2A^{Ry}$, $3A^{Ry}$	*p*(C)	0.127
5A	σ(C1-C3)	5A*, 6A*, 7A* 8A*	σ*(C-C) π*(C-C)	0.053	$4A^{Ry}$, $5A^{Ry}$, $6A^{Ry}$	*p*(C)	0.235
6A	σ(C1-C4)	5A*, 6A*, 7A* 8A*	σ*(C-C) π*(C-C)	0.007	$4A^{Ry}$, $5A^{Ry}$, $6A^{Ry}$	*p*(C)	0.246
7A	σ(C1-C5)	5A*, 6A*, 7A* 8A*	σ*(C-C) π*(C-C)	0.007	$4A^{Ry}$, $5A^{Ry}$, $6A^{Ry}$	*p*(C)	0.246
8A	π(C1-C5)	5A*, 6A*, 7A* 8A*	σ*(C-C) π*(C-C)	0.218	$4A^{Ry}$, $5A^{Ry}$, $6A^{Ry}$	*p*(C)	0.188
1B	σ(C2-C6)	1B*, 2B*, 3B* 4B*	σ*(C-C) p(C)	0.074	$1B^{Ry}$, $2B^{Ry}$, $3B^{Ry}$	*p(C)*	0.238
2B	σ(C2-C8)	1B*, 2B*, 3B* 4B*	σ*(C-C) p(C)	0.082	$1B^{Ry}$, $2B^{Ry}$, $3B^{Ry}$	*p(C)*	0.228
3B	σ(C2-C7)	1B*, 2B*, 3B* 4B*	σ*(C-C) p(C)	0.087	$1B^{Ry}$, $2B^{Ry}$, $3B^{Ry}$	*p(C)*	0.240
4B	σ(C1-C3)	5B*, 6B*, 7B* 8B*	σ*(C-C) p(C)	0.134	$4B^{Ry}$, $5B^{Ry}$, $6B^{Ry}$	*p(C)*	0.280
5B	σ(C1-C4)	5B*, 6B*, 7B* 8B*	σ*(C-C) p(C)	0.072	$4B^{Ry}$, $5B^{Ry}$, $6B^{Ry}$	*p(C)*	0.265
6B	σ(C1-C5)	5B*, 6B*, 7B* 8B*	σ*(C-C) p(C)	0.067	$4B^{Ry}$, $5B^{Ry}$, $6B^{Ry}$	*p(C)*	0.255

Natural Bond Orbital Deletion (NBODel)

The input to calculate the energy deletion of both alpha and beta interactions for **1p-I_3** shown in **Table 3** has the following NBO keywords,

$NBO $END
$DEL
ALPHA
ZERO 2 ATOM BLOCKS
25 BY 25
20 15 64 65 54 55 45 46 41 42 24 60 61 43 44 33 16 17 37 38 47 48 31 32 13
12 49 50 51 66 67 62 63 34 35 23 68 69 70 71 36 58 59 56 57 52 53 39 40 25
25 BY 25
12 49 50 51 66 67 62 63 34 35 23 68 69 70 71 36 58 59 56 57 52 53 39 40 25
20 15 64 65 54 55 45 46 41 42 24 60 61 43 44 33 16 17 37 38 47 48 31 32 13
BETA
ZERO 2 ATOM BLOCKS
25 BY 25
20 15 64 65 54 55 45 46 41 42 24 60 61 43 44 33 16 17 37 38 47 48 31 32 13
12 49 50 51 66 67 62 63 34 35 23 68 69 70 71 36 58 59 56 57 52 53 39 40 25
25 BY 25
12 49 50 51 66 67 62 63 34 35 23 68 69 70 71 36 58 59 56 57 52 53 39 40 25
20 15 64 65 54 55 45 46 41 42 24 60 61 43 44 33 16 17 37 38 47 48 31 32 13
$END

This calculation leads to an interaction energy between the tricyclic structures of 55.4 kcal/mol. Furthermore, all the NBODel analysis were performed at HF/[cc-pVTZ,LANL2TZ(f)]//ωB9X-D/[cc-pVTZ,LANL2TZ(f)].

Natural Resonance Theory (NRT)

The following keyword was used to perform the NRT calculation over **1p-I_3**:

$NBO NRT <12 25 36 70 68 23 49 50 66 62 34 39 52 56 58 20 13 33 43 60 24 15 64 54 45 41 31 47 37 16> MEMORY=40GB NRTRES=40000 NRTE2=1 $END

The numbers following the NRT keyword are the carbon atoms from the tricyclic framework of interest that generate the resonance structures. Calculation performed at HF/[cc-pVTZ,LANL2TZ(f)]//ωB9X-D/[cc-pVTZ,LANL2TZ(f)].

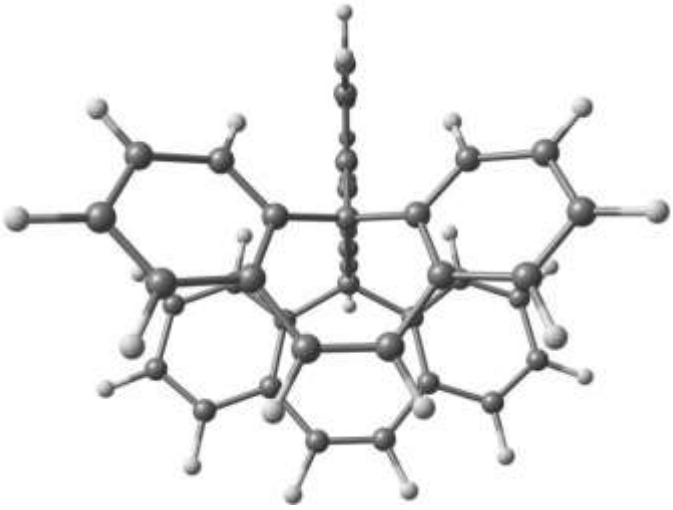
Cartesian Coordinates

Table S4. XYZ cartesian coordinates of the optimized geometries calculated with the long range functional ωB97X-D along with the basis set cc-pVTZ for C, H and LANL2TZ(f) for I.

1

[1]

SCF energy = -1616.03726986 a.u.



6	−2.137870	0.000233	−0.144204
6	−3.490682	0.000309	−0.288060
6	−4.129191	0.000139	−1.530980
6	−5.709511	0.000327	0.157703
1	−6.652693	0.000383	0.681940
6	−1.304062	0.000014	−1.254273
6	−2.384284	0.000366	2.194568
1	−1.985839	0.000370	3.200605
6	−0.004471	0.000052	0.943879
6	0.726238	1.349579	−1.284420
6	−4.377279	0.000400	0.789534
6	0.726143	−1.349689	−1.284312
6	2.287678	2.956792	−2.197682
1	3.237634	3.145292	−2.680834
6	−5.564194	0.000153	−1.192319
1	−6.375726	0.000051	−1.903760
6	0.158006	−0.000017	−0.805160
6	−3.803197	0.000434	2.043684
1	−4.407094	0.000501	2.942384
6	1.977232	−1.553986	1.497371
6	1.948633	−1.622510	−1.916828
6	0.605104	1.262046	1.581748
6	−1.531388	0.000257	1.105465
6	−3.311469	−0.000088	−2.640857
1	−3.721604	−0.000240	−3.642923
6	−1.889838	−0.000132	−2.497352
1	−1.279715	−0.000315	−3.390936
6	−0.098663	2.449629	−1.014475
1	−1.056005	2.285863	−0.546217
6	1.948814	1.622322	−1.916830
6	2.453091	−2.783483	1.961104
1	3.508467	−2.997243	1.850948
6	1.977586	1.553681	1.497268
6	1.471328	4.017855	−1.887034
1	1.776089	5.030345	−2.112522
6	−0.208217	2.217152	2.192846
1	−1.270201	2.054739	2.254643
6	2.287357	−2.957021	−2.197758
1	3.237234	−3.145574	−2.681043
6	2.957062	0.664402	−2.340713
1	3.849917	1.129488	−2.742266
6	1.470978	−4.018016	−1.887008
1	1.775626	−5.030530	−2.112534
6	0.251704	3.753344	−1.288868
1	−0.426170	4.554298	−1.028887
6	0.604815	−1.262050	1.581807
6	−0.208735	−2.216994	2.192867
1	−1.270701	−2.054428	2.254508
6	0.282856	3.412086	2.684144
1	−0.397542	4.119032	3.139115
6	0.251440	−3.753412	−1.288678
1	−0.426455	−4.554323	−1.028618
6	1.627679	3.710002	2.557663
1	2.025262	4.650441	2.913388
6	2.453720	2.783105	1.960903
1	3.509144	2.996613	1.850713
6	2.956972	−0.664693	−2.340718
1	3.849779	−1.129883	−2.742255
6	1.626844	−3.710172	2.557905

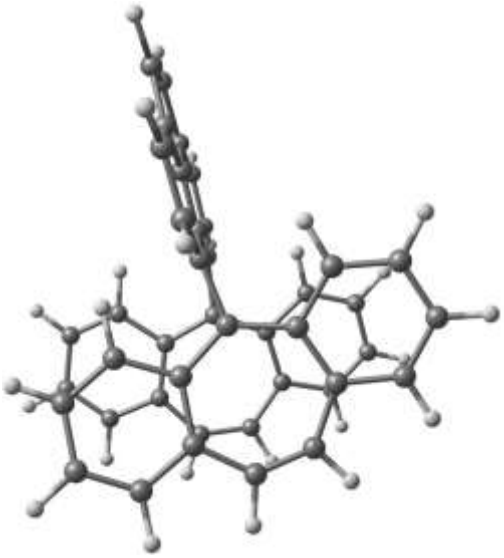
1	2.024257	–4.650616	2.913811
6	–0.098823	–2.449682	–1.014285
1	–1.056136	–2.285831	–0.545998
6	0.282072	–3.411993	2.684272
1	–0.398512	–4.118802	3.139178
6	2.978103	–0.665353	0.928490
1	3.851949	–1.160493	0.522369
6	2.978229	0.664800	0.928420
1	3.852170	1.159729	0.522237

1p

$[1]^{\bullet+}$

(without counterion)

SCF energy = -1615.81855033 a.u.



6	2.041949	–0.000285	–0.000075
6	3.425834	–0.000449	–0.000115
6	4.235904	0.142049	1.143473
6	5.625768	–0.085783	–0.668977
1	6.497376	–0.168912	–1.298578
6	1.414696	0.110267	1.276539
6	2.201595	–0.271129	–2.394598
1	1.715163	–0.345681	–3.358591
6	–0.062540	0.079718	–1.430218
6	–0.832435	1.119145	1.633520
6	4.235808	–0.142989	–1.143772
6	–0.456578	–1.461826	1.530735
6	–2.826193	2.466585	2.037713
1	–3.896832	2.512433	2.182903
6	5.625825	0.084624	0.668589
1	6.497486	0.167602	1.298136
6	–0.062480	–0.079737	1.430201
6	3.617035	–0.298977	–2.351851
1	4.171346	–0.421263	–3.272436
6	–2.245560	–1.210166	–1.810924
6	–1.790475	–1.967864	1.551797
6	–0.456240	1.461896	–1.530787
6	1.414610	–0.110636	–1.276676
6	3.617220	0.298317	2.351571
1	4.171603	0.420624	3.272111
6	2.201788	0.270773	2.394398
1	1.715423	0.345534	3.358408
6	–0.120949	2.346381	1.635710
1	0.941437	2.332580	1.465138
6	–2.245218	1.210677	1.810749
6	–2.826871	–2.465989	–2.037505
1	–3.897496	–2.511574	–2.182887
6	–1.790001	1.968303	–1.552024
6	–2.090778	3.625880	2.078318
1	–2.575533	4.573744	2.264310
6	0.581370	2.435577	–1.574968
1	1.607383	2.112047	–1.585983
6	–1.997509	–3.357474	1.568523
1	–3.017006	–3.717660	1.566056
6	–3.184223	0.128573	1.723914
1	–4.218881	0.443579	1.779930
6	–0.966192	–4.258890	1.611639
1	–1.168858	–5.320014	1.642296
6	–0.719716	3.559392	1.857686
1	–0.120104	4.458292	1.854990
6	–0.832784	–1.118992	–1.633416
6	–0.121644	–2.346437	–1.635174
1	0.940719	–2.332895	–1.464457
6	0.343375	3.781910	–1.631435
1	1.176535	4.468186	–1.684508
6	0.342374	–3.782057	1.631830
1	1.175339	–4.468557	1.685076
6	–0.965065	4.259106	–1.611278

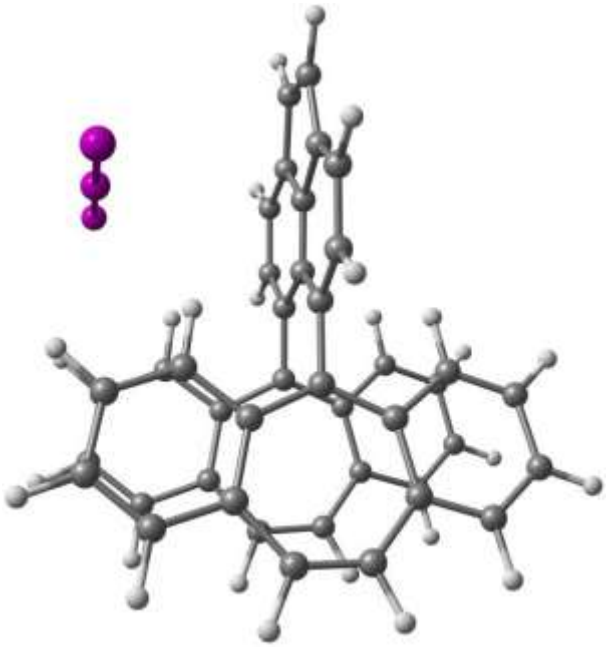
1	–1.167428	5.320294	–1.641728
6	–1.996642	3.357976	–1.568507
1	–3.016040	3.718446	–1.566133
6	–2.994916	–1.191591	1.589436
1	–3.899254	–1.785947	1.544640
6	–2.091803	–3.625522	–2.077494
1	–2.576820	–4.573318	–2.263146
6	0.580750	–2.435796	1.575149
1	1.606857	–2.112573	1.586213
6	–0.720744	–3.559354	–1.856747
1	–0.121405	–4.458434	–1.853623
6	–3.184252	–0.127754	–1.724802
1	–4.218979	–0.442433	–1.781382
6	–2.994626	1.192368	–1.590276
1	–3.898821	1.786979	–1.545982

1p-I_3

$[1]^{\bullet+}$ $[I_3]^-$

(counterion side-on)

SCF energy = -1650.25979905 a.u.



53	–3.359369	0.130975	0.165493
53	–3.636151	–2.776561	0.675391
53	–3.047968	3.009120	–0.314643
6	0.451875	–0.186382	–1.538587
6	–0.534042	–0.187095	–2.511556
6	–0.960101	0.943260	–3.234895
6	–2.284558	–0.818691	–3.865273
1	–3.049684	–1.425050	–4.323089
6	1.077797	1.071491	–1.288936
6	–0.092574	–2.520333	–1.225488
1	0.069554	–3.453123	–0.701357
6	1.744446	–1.548758	0.157543
6	1.676283	1.715484	1.022834
6	–1.325545	–1.297651	–2.861803
6	3.496880	1.227762	–0.784080
6	1.809638	2.561614	3.307506
1	2.414883	2.936597	4.121879
6	–2.070116	0.493656	–4.084089

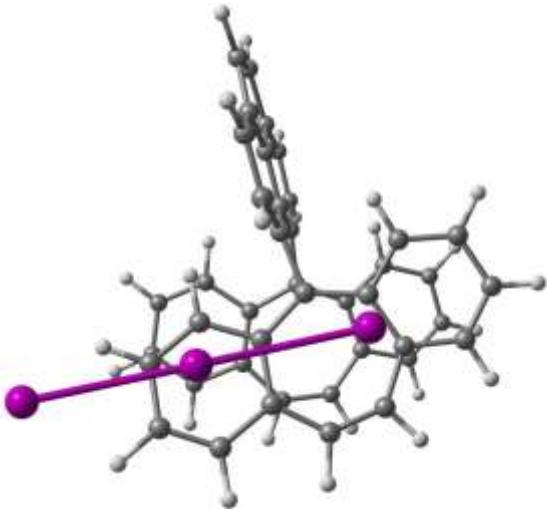
1	–2.632017	1.129212	–4.749644
6	2.152564	1.286867	–0.263633
6	–1.109108	–2.475009	–2.208047
1	–1.706807	–3.356989	–2.388675
6	4.279016	–1.817527	0.348001
6	4.699725	1.608217	–0.119947
6	1.303768	–1.441727	1.523558
6	0.677895	–1.433832	–0.880971
6	–0.352875	2.136947	–2.978224
1	–0.652225	3.053571	–3.466554
6	0.670410	2.174765	–2.002644
1	1.136661	3.127168	–1.786815
6	0.276753	1.637052	1.235632
1	–0.364218	1.288016	0.444211
6	2.456281	2.200393	2.119185
6	5.461727	–2.204896	–0.297794
1	6.395388	–2.076506	0.233124
6	2.134677	–1.202373	2.657681
6	0.447901	2.459515	3.469731
1	–0.012932	2.749596	4.403557
6	–0.087608	–1.537625	1.765518
1	–0.765196	–1.697691	0.945325
6	5.924589	1.474683	–0.793431
1	6.823456	1.780442	–0.275290
6	3.877199	2.387283	2.136390
1	4.250550	2.797429	3.067248
6	6.018848	0.976819	–2.068474
1	6.982374	0.887761	–2.550370
6	–0.324801	1.991610	2.414949
1	–1.398932	1.906221	2.498898
6	3.040425	–1.943763	–0.340435
6	3.097824	–2.472665	–1.655325
1	2.182855	–2.575385	–2.213185
6	–0.632676	–1.460059	3.021464
1	–1.702672	–1.572132	3.130818
6	4.855625	0.593092	–2.726904
1	4.898223	0.189177	–3.728241
6	0.187992	–1.215251	4.115193
1	–0.229172	–1.127357	5.108706
6	1.542982	–1.076438	3.918999
1	2.185122	–0.866893	4.764079
6	4.810688	2.144074	1.205767
1	5.826260	2.386682	1.494579
6	5.471377	–2.742618	–1.561153
1	6.403191	–3.045821	–2.017641
6	3.643426	0.722035	–2.102359
1	2.762805	0.419284	–2.642405
6	4.266134	–2.885569	–2.241101
1	4.243744	–3.305734	–3.236782
6	4.455676	–1.271439	1.667274
1	5.489247	–1.073311	1.925091
6	3.560764	–1.017020	2.629893
1	3.971327	–0.641831	3.559910

1p-I_3-2

$[1]^{\bullet+}$ $[I_3]^-$

(counterion above-the-plane)

SCF energy = -1650.25676637 a.u.



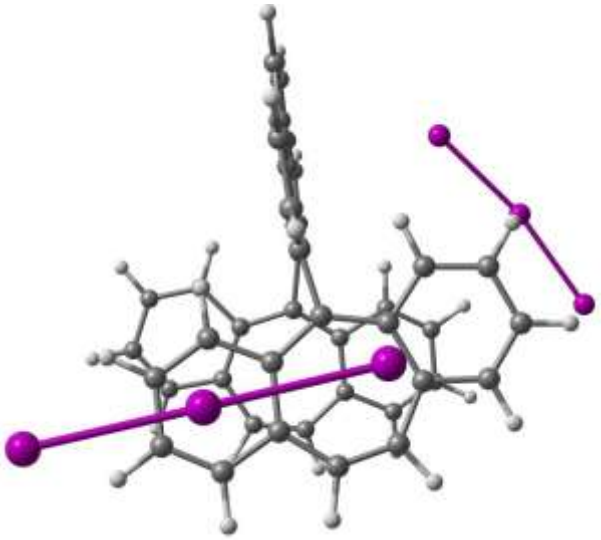
53	3.552021	0.726479	0.281128
53	1.909957	3.182044	0.717382
53	5.006625	–1.749132	–0.196903
6	–2.209453	–0.998624	1.779437
6	–2.328311	–1.395760	3.102208
6	–3.438114	–2.068616	3.648720
6	–1.907310	–1.774330	5.332343
1	–1.405321	–1.788112	6.286993
6	–3.287693	–1.358649	0.913203
6	–0.048019	–0.101150	2.423591
1	0.845988	0.449176	2.158365
6	–0.821960	0.389923	0.138267
6	–3.911437	–0.061008	–1.130416
6	–1.356454	–1.190362	4.102125
6	–2.509027	–2.273841	–1.239164
6	–4.666362	1.475104	–2.865679
1	–4.636615	1.781595	–3.903085
6	–3.127825	–2.284646	5.068112
1	–3.778776	–2.773788	5.775714
6	–3.190966	–1.182013	–0.570665
6	–0.197360	–0.556085	3.755452
1	0.598507	–0.372280	4.464205
6	0.455585	0.180547	–2.060495
6	–2.081168	–2.303305	–2.595955
6	–1.444876	1.677406	0.058629
6	–1.012911	–0.286146	1.461136
6	–4.486745	–2.353737	2.819645
1	–5.375663	–2.861976	3.169263
6	–4.382745	–1.997022	1.455010
1	–5.189700	–2.271674	0.787858
6	–4.690827	0.718194	–0.242172
1	–4.703584	0.458185	0.802653
6	–3.892572	0.374057	–2.486328
6	1.375097	–0.590565	–2.794196
1	1.718603	–0.203763	–3.743121
6	–1.509636	2.521175	–1.089314
6	–5.446817	2.181500	–1.977142
1	–6.033263	3.025413	–2.311778
6	–2.073104	2.169723	1.239149
1	–2.016243	1.593428	2.144915
6	–1.361128	–3.406909	–3.067777
1	–1.029148	–3.391710	–4.097355
6	–3.076457	–0.180204	–3.544833
1	–3.100873	0.401362	–4.458852
6	–1.067302	–4.497597	–2.282861
1	–0.512710	–5.332001	–2.688006
6	–5.440934	1.797935	–0.644491
1	–6.015798	2.346817	0.088469
6	0.027304	–0.288208	–0.778299
6	0.520728	–1.561859	–0.373089
1	0.205243	–1.964682	0.572429
6	–2.719213	3.368693	1.291794
1	–3.152174	3.701310	2.224195
6	–1.500789	–4.498479	–0.964573
1	–1.294754	–5.340345	–0.318312
6	–2.817781	4.159049	0.144136
1	–3.338263	5.106077	0.171679
6	–2.229378	3.731209	–1.010316
1	–2.280275	4.347667	–1.896596
6	–2.313677	–1.274498	–3.583810
1	–1.803614	–1.452521	–4.523153

6	1.850154	–1.790404	–2.341887
1	2.579265	–2.341849	–2.917388
6	–2.185505	–3.417188	–0.465027
1	–2.491856	–3.458489	0.566123
6	1.394543	–2.291858	–1.121242
1	1.756945	–3.239644	–0.754085
6	0.006265	1.353419	–2.722443
1	0.421637	1.483757	–3.713801
6	–0.856216	2.311957	–2.332365
1	–1.041085	3.089350	–3.062987

1pp-I_3

$[1]^{+2}[I_3]_2^{2-}$

SCF energy = -1684.47839284 a.u.



53	–5.530014	–0.309548	–0.590216
53	–4.191087	1.768414	–2.183700
53	–6.307374	–2.491258	1.240204
53	4.844880	–1.587212	–1.165598
53	7.181504	–0.067579	–0.260828
53	2.358613	–2.997254	–1.912126
6	–0.139904	2.246872	–0.627597
6	–0.435533	3.075388	–1.698799
6	–0.253401	2.077478	1.925825
6	–0.724381	2.642511	0.618593
6	0.920534	2.730653	2.435312
6	–1.044211	1.041375	2.488222
6	–1.305363	4.184476	–1.657281
6	–0.734399	0.256082	3.654749
6	1.691961	2.344094	3.575876
6	–1.602779	3.700176	0.655665
1	–2.035001	3.976915	1.608844
6	–1.925121	4.478764	–0.478721
1	–2.640944	5.283008	–0.385503
6	–2.261376	0.724540	1.811683
1	–2.530426	1.261206	0.915215
6	0.434180	0.349694	4.450710
1	0.498663	–0.402067	5.227376
6	1.460556	1.225051	4.415465
1	2.224639	1.069697	5.166354
6	1.386109	3.877227	1.723159
1	0.848212	4.210388	0.854057
6	–1.633409	–0.747526	4.062265
1	–1.379954	–1.334252	4.934120
6	–1.354266	4.723289	–3.022414
1	–1.950643	5.567402	–3.329231
6	–3.115945	–0.238545	2.258764
1	–4.029164	–0.437223	1.719412
6	2.831676	3.100241	3.925543
1	3.405940	2.782512	4.784208
6	2.482313	4.594059	2.103046
1	2.777035	5.460613	1.529062
6	–2.802045	–0.989207	3.395413
1	–3.484460	–1.760558	3.726072
6	3.221064	4.203765	3.223697
1	4.095598	4.762095	3.526707
6	0.888682	–0.009326	0.028464
6	0.683673	1.118101	–0.940278
6	–0.158542	–0.979963	–0.000762
6	2.079549	0.057054	0.796909
6	0.045787	2.905551	–3.012433
6	2.514742	–0.874453	1.795898
6	–0.288596	–2.124046	0.853847
6	1.187028	0.967669	–2.209769
1	1.791279	0.093526	–2.420985
6	0.886408	1.861135	–3.265392
1	1.296366	1.671057	–4.247584
6	2.946826	1.165866	0.546183
1	2.673619	1.871477	–0.218320
6	1.826300	–2.033727	2.221857

1	2.345674	−2.599827	2.984832
6	0.633825	−2.544960	1.840791
1	0.342803	−3.453466	2.353341
6	−1.179532	−0.807554	−0.978664
1	−1.142560	0.024493	−1.658425
6	3.739312	−0.640450	2.460907
1	4.066034	−1.368347	3.189854
6	−0.558479	3.978904	−3.813908
1	−0.392589	4.125902	−4.869198
6	4.110956	1.363888	1.218656
1	4.740929	2.204902	0.971809
6	−1.414786	−2.959322	0.716281
1	−1.506337	−3.804360	1.384057
6	−2.226652	−1.670421	−1.116199
1	−2.956065	−1.495316	−1.891717
6	4.521495	0.443633	2.193050
1	5.465757	0.576699	2.700075
6	−2.367105	−2.751916	−0.242286
1	−3.222947	−3.408007	−0.318415