Table S1. Topological Properties of X-**1** and X-**2** for X = H, NH_2 and NO_2 at RHF/6-31G*.

#	A	B	r_A	r_B	F	ρ	λ_1	λ_2	λ_3	ε
					H-**1**					
1	C1	C5	0.763	0.628	0.584	0.322	-0.694	-0.560	0.210	0.240
2	C5	C7	0.728	0.651	0.528	0.329	-0.712	-0.579	0.247	0.230
3	C7	C8	0.690	0.702	0.496	0.325	-0.700	-0.589	0.275	0.188
4	C5	H10	0.706	0.369	0.657	0.291	-0.813	-0.806	0.477	0.008
5	C7	H12	0.704	0.371	0.654	0.291	-0.816	-0.804	0.478	0.015
6	C8	H13	0.707	0.370	0.656	0.293	-0.824	-0.822	0.484	0.002
7	C1	N2	0.434	0.986	0.306	0.216	-0.290	-0.230	1.245	0.258
8	N2	N3	0.604	0.472	0.561	0.680	-1.560	-1.505	0.434	0.036
9[b]	C1	C8	1.317	1.382	0.480	0.020	-0.014	0.086	0.096	-----
					H-**2**					
1	C1	C2	0.876	0.455	0.658	0.341	-0.670	-0.572	0.450	0.170
2	C2	C4	0.753	0.660	0.533	0.298	-0.606	-0.505	0.249	0.200
3	C4	C6	0.717	0.672	0.516	0.326	-0.703	-0.576	0.265	0.219
4	C2	H7	0.724	0.347	0.676	0.287	-0.831	-0.823	0.468	0.009
5	C4	H9	0.712	0.362	0.663	0.292	-0.833	-0.822	0.481	0.014
6	C6	H11	0.707	0.366	0.659	0.294	-0.832	-0.821	0.480	0.013
6[b]	C1	C4	1.138	1.328	0.461	0.025	-0.019	0.083	0.120	------
					NH_2-**1**					
1	C1	C5	0.741	0.664	0.527	0.314	-0.676	-0.556	0.263	0.217
2	C5	C7	0.718	0.640	0.529	0.341	-0.749	-0.567	0.225	0.321
3	C7	C8	0.661	0.760	0.465	0.311	-0.668	-0.568	0.266	0.175
4	C5	H10	0.704	0.370	0.656	0.293	-0.820	-0.817	0.479	0.004
5	C7	H12	0.695	0.378	0.647	0.289	-0.799	-0.777	0.470	0.029
6	C8	N13	0.439	0.889	0.330	0.346	-0.804	-0.798	0.804	0.008
7	N13	H14	0.767	0.229	0.770	0.342	-1.388	-1.333	0.935	0.041
8	C1	N2	0.423	0.948	0.309	0.243	-0.422	-0.250	1.554	0.692
9	N2	N3	0.618	0.465	0.571	0.665	-1.534	-1.422	0.413	0.079
10	C1	C8	1.358	1.396	0.493	0.019	-0.013	0.085	0.088	-----
					NH_2-**2**					
1	C1	C2	0.866	0.466	0.650	0.339	-0.667	-0.585	0.308	0.142
2	C2	C4	0.754	0.643	0.540	0.305	-0.629	-0.494	0.228	0.272

3	C4	C6	0.687	0.724	0.487	0.316	-0.687	-0.561	0.283	0.225
4	C2	H7	0.722	0.350	0.674	0.288	-0.833	-0.828	0.471	0.006
5	C4	H9	0.704	0.370	0.655	0.289	-0.811	-0.789	0.475	0.028
6	C6	N11	0.453	0.893	0.336	0.337	-0.776	-0.774	0.542	0.043
7	N11	H12	0.748	0.230	0.765	0.342	-1.381	-1.319	0.923	0.047
8[b]	C1	C6	1.172	1.347	0.465	0.023	-0.017	0.084	0.107	-----
					NO_2-**1**					
1	C1	C5	0.767	0.619	0.553	0.325	-0.702	-0.565	0.206	0.244
2	C5	C7	0.716	0.664	0.519	0.329	-0.710	-0.586	0.259	0.213
3	C7	C8	0.658	0.726	0.475	0.331	-0.724	-0.593	0.258	0.220
4	C5	H10	0.708	0.365	0.660	0.293	-0.826	-0.818	0.477	0.010
5	C7	H12	0.718	0.353	0.670	0.296	-0.853	-0.845	0.479	0.010
6	C8	N13	0.522	0.948	0.355	0.279	-0.601	-0.583	0.211	0.030
7	N13	O14	0.576	0.611	0.485	0.556	-1.442	-1.274	1.310	0.132
8	C1	N2	0.435	0.989	0.306	0.215	-0.283	-0.251	1.204	0.127
9	N2	N3	0.601	0.475	0.559	0.680	-1.556	-1.513	0.450	0.028
10	C1	C8	1.313	1.353	0.492	0.021	-0.015	0.086	0.097	-----
					NO_2-**2**					
1	C1	C2	0.650	0.453	0.589	0.341	-0.672	-0.572	0.472	0.175
2	C2	C4	0.540	0.670	0.446	0.301	-0.615	-0.516	0.259	0.191
3	C4	C6	0.487	0.700	0.410	0.330	-0.724	-0.578	0.272	0.252
4	C2	H7	0.674	0.343	0.662	0.287	-0.836	-0.827	0.467	0.010
5	C4	H9	0.655	0.344	0.655	0.294	-0.860	-0.853	0.479	0.009
6	C6	N11	0.336	0.939	0.264	0.283	-0.627	-0.576	0.205	0.088
7	N11	O12	0.765	0.610	0.556	0.557	-1.443	-1.274	1.317	0.133
8[b]	C1	C6	0.465	1.299	0.264	0.025	-0.019	0.082	0.120	-----

(a) The r_A and r_B values are the distances in Ångstroms between the critical point and the atoms A and B, respectively. F is defined as the ratio $r_A/(r_A+r_B)$. The value of the electron density at the critical point, ρ, is given in e au^{-3}. The curvatures of the electron density at the location of the critical points, λ_i, are given in e au^{-5}. The ellipticity, ε, is defined as $\varepsilon = \lambda_1/\lambda_2 - 1$. These points are (3,-1) *ring* critical points. All other critical points are (3,-1) *bond* critical points.

(b) Ring critical points are characterized by their location with respect to C1, the carbon that carries the diazonio function, and the "*para*-carbon".

Table S2. Topological Properties of H-**1** and H-**2** at the levels MP2(full)/6-31G* and CISD(full)/6-31G*//RHF/6-31G*.

#	A	B	r_A	r_B	F	ρ	λ_1	λ_2	λ_3	ε
				H-**1**, MP2						
1	C1	C5	0.753	0.647	0.538	0.303	-0.624	-0.508	0.294	0.226
2	C5	C7	0.714	0.676	0.514	0.312	-0.646	-0.535	0.318	0.207
3	C7	C8	0.705	0.696	0.503	0.310	-0.639	-0.543	0.328	0.176
4	C5	H10	0.720	0.366	0.663	0.276	-0.767	-0.757	0.503	0.013
5	C7	H12	0.720	0.366	0.663	0.279	-0.778	-0.771	0.508	0.008
6	C8	H13	0.720	0.366	0.663	0.279	-0.778	-0.772	0.510	0.007
7	C1	N2	0.439	0.948	0.316	0.245	-0.359	-0.320	1.053	0.124
8	N2	N3	0.613	0.523	0.539	0.577	-1.239	-1.236	0.866	0.003
9[b]	C1	C8	1.328	1.389	0.489	0.020	-0.015	0.082	0.094	-----
				H-**2**, MP2						
1	C1	C2	0.792	0.536	0.596	0.339	-0.650	-0.537	0.118	0.212
2	C2	C4	0.749	0.688	0.521	0.268	-0.506	-0.427	0.311	0.184
3	C4	C6	0.717	0.677	0.514	0.312	-0.645	-0.531	0.319	0.216
4	C2	H7	0.737	0.346	0.680	0.270	-0.775	-0.766	0.488	0.011
5	C4	H9	0.729	0.359	0.670	0.275	-0.778	-0.766	0.505	0.016
6	C6	H11	0.723	0.362	0.666	0.278	-0.778	-0.770	0.505	0.011
6[b]	C1	C6	1.161	1.318	0.468	0.027	-0.023	0.080	0.126	-----
				H-**1**, CISD						
1	C1	C5	0.754	0.636	0.542	0.317	-0.673	-0.544	0.258	0.237
2	C5	C7	0.719	0.659	0.522	0.325	-0.691	-0.566	0.282	0.221
3	C7	C8	0.693	0.698	0.498	0.320	-0.679	-0.574	0.304	0.183
4	C5	H10	0.707	0.367	0.658	0.289	-0.809	-0.802	0.497	0.009
5	C7	H12	0.705	0.367	0.658	0.290	-0.816	-0.806	0.500	0.012
6	C8	H13	0.707	0.367	0.658	0.291	-0.820	-0.818	0.504	0.003
7	C1	N2	0.439	0.975	0.310	0.225	-0.304	-0.253	1.097	0.204
8	N2	N3	0.596	0.481	0.554	0.672	-1.624	-1.488	0.544	0.024
9[b]	C1	C8	1.317	1.379	0.489	0.021	-0.015	0.086	0.098	-----

				H-2, CISD						
1	C1	C2	0.845	0.484	0.636	0.341	-0.652	-0.544	0.195	0.199
2	C2	C4	0.754	0.683	0.524	0.277	-0.539	-0.452	0.295	0.191
3	C4	C6	0.719	0.674	0.516	0.317	-0.669	-0.549	0.300	0.220
4	C2	H7	0.734	0.349	0.678	0.275	-0.787	-0.779	0.488	0.010
5	C4	H9	0.725	0.363	0.666	0.279	-0.789	-0.777	0.505	0.015
6	C6	H11	0.719	0.366	0.663	0.281	-0.789	-0.779	0.504	0.013
6[b]	C1	C6	1.151	1.328	0.464	0.026	-0.020	0.081	0.121	-----

(a) See footnotes to preceding table.

Table S3. Integrated Properties of X-**1** and X-**2** for X = H, NH_2, and NO_2 at RHF/6-31G*.

Atom	Charge	π-Pop.	μ	KE	Charge	π-Pop.	μ	KE
	H-**1**				H-**2**			
C_{ipso}	0.138	1.190	0.740	37.75819	-0.735	1.415	0.090	38.48871
C_{ortho}	0.076	0.896	-0.357	37.83443	0.348	0.882	0.787	37.59906
C_{meta}	0.063	0.937	0.217	37.82893	0.051	0.913	0.286	37.78281
C_{para}	0.018	0.844	-0.121	37.86649	0.079	0.913	0.214	37.79210
H_{ortho}	0.114	0.018	0.126	0.57008	0.222	0.015	0.120	0.51488
H_{meta}	0.103	0.019	0.126	0.57627	0.145	0.018	0.124	0.55798
H_{para}	0.106	0.017	-0.126	0.57705	0.124	0.018	0.125	0.56823
N_α	-0.540	1.293	0.345	54.99035				
N_β	0.558	0.918	-0.883	53.93115				
Σ	0.992	8.006		338.74265	1.000	6.000		229.75850
Σ(H)	0.540	0.091		2.86975	0.858	0.084		2.71395
Σ(C)	0.434	5.700		226.95140	0.142	5.918		227.04455
o-CH	0.190	0.914		38.40451	0.570	0.897		38.11394
m-CH	0.166	0.956		38.40520	0.196	0.931		38.34079
p-CH	0.124	0.861		38.44354	0.203	0.931		38.36033
Ph	0.974	5.791		229.82115				
N_2	0.018	2.211		108.92150				
IOP	0.518	3.018		114.56721	0.405	3.209		114.71659
MPR	0.350	2.756		114.67689	0.471	2.775		114.47368
	NH_2-**1**				NH_2-**2**			
C_{ipso}	0.249	1.214	0.723	37.67211	-0.732	1.481	0.124	38.47550
C_{ortho}	0.058	0.873	-0.271	37.85447	0.345	0.858	-0.756	37.61938
C_{meta}	0.075	1.039	-0.231	37.81976	0.068	1.032	0.274	37.77225
C_{para}	0.693	0.699	-0.872	37.43969	0.718	0.787	-0.760	37.39989
H_{orthe}	0.106	0.017	-0.129	0.57606	0.209	0.015	-0.120	0.52208
H_{meta}	0.078	0.023	-0.126	0.58668	0.116	0.022	-0.127	0.56971
$N(NH_2)$	-1.447	1.820	-0.371	55.20814	-1.428	1.868	-0.239	55.12991
$H(NH_2)$	0.486	0.012	0.161	0.40741	0.481	0.013	-0.163	0.40967
N_α	-0.627	1.330	0.362	55.06142				
N_β	0.522	1.008	-0.923	53.92178				
Σ	0.996	9.999		393.79190	0.996	8.016		284.79148

Σ(H)	0.368	0.080	2.32548	0.650	0.074	2.18358
Σ(C)	1.208	5.737	189.02057	0.812	6.048	226.65865
o-CH	0.164	0.890	38.43053	0.554	0.873	38.14146
m-CH	0.153	1.062	38.40644	0.184	1.054	38.34196
p-CX	0.218	2.543	93.46265	0.252	2.681	93.34914
X-Ph	1.101	7.661	284.80870			
N_2	-0.105	2.338	108.98320			
IOP	0.577	2.994	114.53317	0.376	3.227	114.75842
MPR	0.999	2.823	114.25257	1.086	2.895	114.08381

	NO_2-**1**				NO_2-**2**			
C_{ipso}	0.134	1.168	0.757	37.77850	-0.718	1.388	0.115	38.50883
C_{ortho}	0.108	0.896	-0.358	37.82732	0.373	0.874	-0.783	37.61114
C_{meta}	0.108	0.883	-0.296	37.84273	0.099	0.861	-0.303	37.80641
C_{para}	0.293	0.963	-0.573	37.74509	0.367	1.014	-0.508	37.69007
H_{ortho}	0.130	0.018	-0.124	0.56428	0.240	0.014	-0.118	0.50630
H_{meta}	0.174	0.016	-0.120	0.54915	0.215	0.014	-0.118	0.52879
N(NO_2)	0.465	1.051	-0.847	54.08742	0.475	1.055	-0.820	54.06144
O(NO_2)	-0.498	1.506	-0.302	75.04481	-0.492	1.507	-0.302	75.01516
N_α	-0.530	1.291	0.346	54.98831				
N_β	0.577	0.894	-0.867	53.92715				
Σ	0.983	12.005		542.18305	0.994	9.997		433.19594
Σ(H)	0.608	0.068		2.22686	0.910	0.056		2.07018
Σ(C)	0.859	5.689		226.86369	0.593	5.872		227.03400
o-CH	0.238	0.914		38.39160	0.613	0.888		38.11744
m-CH	0.282	0.899		38.39188	0.314	0.875		38.33520
p-CX	-0.238	5.026		241.92213	-0.142	5.083		241.78183
X-Ph	0.936	9.820		433.26759				
N_2	0.047	2.185		108.91546				
IOP	0.610	2.996		114.56170	0.508	3.164		114.74371
MPR	0.857	2.761		114.52885	0.995	2.764		114.36047

(a) Charges and π-populations are given in electrons and dipole moments and integrated kinetic energies (KE, corrected for the virial defect of the wave function) are given in atomic units.

(b) IOP = Σ (C_{ipso} and both *o*-CH). MPR = Σ (C_{para} and both *m*-CH).

Table S4. Integrated Properties of H-**1** and H-**2** at the levels MP2(full)/6-31G* and CISD(full)/6-31G*//RHF/6-31G*.

Atom	Charge	μ	KE	Charge	μ	KE
	H-**1** at MP2			H-**2** at MP2		
C_{ipso}	0.269	0.676	37.87060	-0.273	0.139	38.26927
C_{ortho}	0.011	-0.316	38.03449	0.110	0.548	37.91067
C_{meta}	0.005	0.221	38.04457	-0.005	0.274	37.96371
C_{para}	0.004	0.192	38.04483	0.025	0.261	37.97225
H_{ortho}	0.147	-0.143	0.54837	0.256	0.128	0.49300
H_{meta}	0.141	-0.143	0.55404	0.183	0.138	0.53301
H_{para}	0.134	0.143	0.55682	0.162	0.139	0.54240
N_α	-0.374	0.478	55.02630			
N_β	0.363	-0.733	54.27574			
Σ	0.992		340.13723	1.002		230.58470
Σ(H)	0.710		2.76164	1.040		2.59442
Σ(C)	0.297		228.07355	-0.038		227.99028
o-CH	0.158		38.58286	0.366		38.15367
m-CH	0.146		38.59861	0.178		38.12971
p-CH	0.130		38.60165	0.187		38.51465
Ph	1.003		230.83519			
N_2	-0.011		109.30204			
IOP	0.585			0.459		
MPR	0.288			0.381		
	H-**1** at CISD			H-**2** at CISD		
C_{ipso}	0.187	0.689	37.80802	-0.530	0.040	38.43536
C_{ortho}	0.049	-0.321	37.92837	0.249	0.686	37.76101
C_{meta}	0.038	0.217	37.92884	0.009	0.267	37.89700
C_{para}	0.011	0.143	37.94790	0.049	0.245	37.90821
H_{ortho}	0.124	-0.133	0.56963	0.243	0.121	0.50360
H_{meta}	0.116	-0.134	0.57492	0.166	0.129	0.54584
H_{para}	0.115	0.133	0.57687	0.147	0.130	0.55435
N_α	-0.460	0.395	55.04035			

N_β	-0.493	-0.844	54.09264		
Σ	1.000		339.46930	1.000	230.31282
Σ(H)	0.595		2.86597	0.965	2.65323
Σ(C)	0.372		227.47034	0.035	227.65959
o-CH	0.173		38.49800	0.492	37.76101
m-CH	0.154		38.50376	0.175	37.89700
p-CH	0.126		38.52477	0.196	38.46256
Ph	0.967		230.33631		
N_2	0.033		109.13299		
IOP	0.533			0.454	
MPR	0.423			0.399	

(b) See footnotes to proceeding table.