Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Hidden aspects of the Structural Theory of chemistry: The MC-QTAIM analysis reveals "alchemical" transformation from a triatomic to a diatomic structure

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Table S1- Some results of the topological analysis on the *XCN* series of species including the Gamma density, the combined Lagrangian kinetic energy density (denoted as G), the Laplacian of the Gamma density (denoted as Lap. Γ), computed at the (3, -3) CP on carbon and nitrogen clamped nuclei and the (3, -1) CP connecting these two CPs. The line between $m_X = 80m_e$ and $m_X = 85m_e$ is the border between triatomic and diatomic structures. All results are given in atomic units.

	Gamma			**G**			**Lap. Γ**		
X-mass	**N-(3, -3)**	**LCP**	**C-(3,-3)**	**N-(3, -3)**	**LCP**	**C-(3,-3)**	**N-(3, -3)**	**LCP**	**C-(3,-3)**
1	196.5	0.520	121.4	17.1	1.046	5.0	-1476301	-0.090	-670837
25	196.9	0.522	120.9	17.0	1.271	5.4	-1480090	0.998	-667666
50	196.9	0.523	120.9	17.0	1.276	5.5	-1480078	1.011	-667525
60	196.9	0.523	120.9	17.0	1.276	5.5	-1480074	1.011	-667487
65	196.9	0.523	120.9	17.0	1.276	5.5	-1480030	1.007	-667423
70	196.9	0.523	120.9	17.0	1.276	5.5	-1480016	1.008	-667417
75	196.9	0.523	120.9	17.0	1.276	5.5	-1480008	1.008	-667414
80	196.9	0.523	120.9	17.0	1.276	5.5	-1480004	1.008	-667411
85	196.9	0.523	120.9	17.0	1.276	5.5	-1479999	1.009	-667409
100	196.9	0.523	120.9	17.0	1.276	5.5	-1479990	1.010	-667406
200	196.9	0.524	120.9	17.0	1.278	5.5	-1479966	1.015	-667399
600	196.9	0.524	120.9	17.0	1.279	5.6	-1479945	1.018	-667412
1000	196.9	0.524	120.9	17.0	1.280	5.6	-1479935	1.019	-667424
1400	196.9	0.524	120.9	17.0	1.280	5.6	-1479931	1.019	-667434
1836	196.9	0.524	120.9	17.0	1.280	5.6	-1479929	1.019	-667441

Table S2- Some results of the topological analysis on the *CNX* series of species including the Gamma density, the combined Lagrangian kinetic energy density (denoted as G), the Laplacian of the Gamma density (denoted as Lap. Γ), computed at the (3, -3) CP on carbon and nitrogen clamped nuclei and the (3, -1) CP connecting these two CPs. The line between $m_X = 405m_e$ and $m_X = 410m_e$ is the border between triatomic and diatomic structures. All results are given in atomic units.

	Gamma			**G**			**Lap. Γ**		
X-mass	**C-(3,-3)**	**LCP**	**N-(3, -3)**	**C-(3,-3)**	**LCP**	**N-(3, -3)**	**C-(3,-3)**	**LCP**	**N-(3, -3)**
25	121.6	0.488	195.7	4.7	1.015	18.1	-671651	0.210	-1469770
50	121.6	0.486	195.6	4.6	1.016	18.2	-671610	0.245	-1469217
100	121.7	0.481	195.7	4.6	1.019	18.3	-672369	0.330	-1470200
200	121.6	0.482	195.7	4.6	1.016	18.4	-671676	0.301	-1470216
300	121.6	0.481	195.7	4.6	1.016	18.4	-671648	0.309	-1470135
350	121.6	0.481	195.7	4.6	1.016	18.4	-671629	0.312	-1470117
385	121.6	0.479	195.6	4.5	1.045	18.4	-671897	0.487	-1468964
400	121.6	0.479	195.6	4.5	1.045	18.4	-671893	0.488	-1468955
405	121.6	0.479	195.6	4.5	1.045	18.4	-671893	0.488	-1468952
410	121.6	0.479	195.6	4.5	1.045	18.4	-671894	0.489	-1468950
425	121.6	0.479	195.6	4.5	1.045	18.5	-671893	0.489	-1468940
500	121.6	0.478	195.6	4.5	1.045	18.5	-671896	0.492	-1468903
600	121.6	0.478	195.6	4.5	1.045	18.5	-671893	0.496	-1468862
1000	121.6	0.478	195.6	4.5	1.043	18.5	-671906	0.502	-1468815
1400	121.6	0.477	195.6	4.5	1.044	18.5	-671911	0.506	-1468767
1836	121.6	0.477	195.6	4.5	1.044	18.5	-671916	0.509	-1468737

Table S3- The separate electronic and PCP contributions to the Gamma density, the combined Lagrangian kinetic energy density (denoted as G), the Laplacian of the Gamma density (denoted as Lap. Γ) all computed at the (3, -3) CP located in the *X* basin and at the (3, -1) linking the (3, -3) CP on carbon nucleus and the (3, -3) CP within the *X* basin the for the *XCN* series of species. All results are given in atomic units.

	Gamma*		**G**		**Laplacian of Gamma***	
X-mass	**(3, -1)**	**X-(3, -3)**	**(3, -1)**	**X-(3, -3)**	**(3, -1)**	**X-(3, -3)**
electronic						
85	0.181	0.179	0.007	0.007	-1.061	-1.087
100	0.194	0.182	0.007	0.007	-1.071	-1.288
200	0.226	0.211	0.007	0.008	-1.207	-2.099
600	0.255	0.257	0.011	0.008	-1.125	-3.682
1000	0.263	0.276	0.012	0.009	-1.067	-4.498
1400	0.267	0.288	0.013	0.009	-1.047	-5.046
1836	0.270	0.296	0.014	0.009	-1.037	-5.481
PCP						
85	0.016	0.018	0.040	0.038	-0.302	-0.396
100	0.010	0.023	0.046	0.035	-0.074	-0.730
200	0.002	0.028	0.038	0.038	0.133	-1.647
600	0.000	0.028	0.002	0.052	0.013	-3.538
1000	0.000	0.027	0.000	0.062	0.001	-4.674
1400	0.000	0.026	0.000	0.070	0.000	-5.519
1836	0.000	0.026	0.000	0.078	0.000	-6.249

* The PCP's contribution to the Gamma density and its Laplacian is the mass scaled one-particle density and its Laplacian (see section 2 of paper for details).

Table S4- The separate electronic and PCP contributions to the Gamma density, the combined Lagrangian kinetic energy density (denoted as G), the Laplacian of the Gamma density (denoted as Lap. Γ) all computed at the (3, -3) CP located in the *X* basin and at the (3, -1) linking the (3, -3) CP on nitrogen nucleus and the (3, -3) CP within the *X* basin for the *CNX* series of species. All results are given in atomic units.

	Gamma*		**G**		**Laplacian of Gamma***	
X-mass	**(3, -1)**	**X-(3, -3)**	**(3, -1)**	**X-(3, -3)**	**(3, -1)**	**X-(3, -3)**
electronic						
410	0.255	0.254	0.018	0.018	-2.566	-2.594
425	0.258	0.253	0.018	0.018	-2.544	-2.697
500	0.267	0.257	0.018	0.018	-2.605	-3.005
600	0.276	0.263	0.018	0.018	-2.703	-3.328
1000	0.294	0.280	0.018	0.019	-2.961	-4.208
1400	0.304	0.291	0.019	0.019	-3.021	-4.801
1836	0.311	0.299	0.020	0.019	-2.913	-5.279
PCP						
410	0.015	0.016	0.110	0.108	-0.713	-0.823
425	0.013	0.017	0.114	0.105	-0.481	-1.090
500	0.009	0.020	0.120	0.104	-0.135	-1.611
600	0.006	0.021	0.120	0.106	0.071	-2.054
1000	0.003	0.022	0.099	0.119	0.319	-3.163
1400	0.001	0.022	0.066	0.131	0.292	-3.925
1836	0.000	0.021	0.032	0.143	0.168	-4.570

* The PCP's contribution to the Gamma density and its Laplacian is the mass scaled one-particle density and its Laplacian (see section 2 of paper for details).