Copper Catalyzed Cycloaddition Reaction of Azidomethyl Benzene With 2,2-Di(prop-2-yn-1-yl)propane-1,3-diol: DFT and QTAIM Investigation

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Table S1. Topological parameters of some selected BCPs and RCPs related to product-1, via the QTAIM approach at M06/6-311G** calculated wave function of electron density. Note that numbering of atoms is in accordance with Fig. 4

	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b	$\lvert V_b\rvert/G_b$
BCPs						
C14-C15	0.317	-0.859	0.113	-0.442	-0.328	3.884
C14–N16	0.328	-0.899	0.301	-0.827	-0.526	2.747
C15-N18	0.312	-0.294	0.426	-0.926	-0.499	2.172
N16-N17	0.425	-0.968	0.243	-0.729	-0.485	2.993
N17-N18	0.387	-0.790	0.219	-0.636	-0.417	2.899
N18-C19	0.259	-0.632	0.202	-0.562	-0.360	2.782
C28-H34	0.011	0.040	0.010	-0.008	0.001	0.830
O32-H40	0.016	0.059	0.013	-0.012	0.000	0.931
RCPs						
RCP1	0.006	0.032	0.006	-0.005	0.001	0.785
RCP2	0.011	0.053	0.011	-0.008	0.002	0.793
RCP3	0.021	0.167	0.032	-0.024	0.015	0.859
RCP4	0.056	0.506	0.110	-0.095	0.008	0.731

Table S2. Topological parameters of some selected BCPs and RCPs related to product-2, via the QTAIM approach at M06/6-311G** calculated wave function of electron density. Note that numbering of atoms is in accordance with Fig. 4

	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b	$\lvert V_b\rvert/G_b$
BCPs						
H8-H51	0.003	0.012	0.002	-0.001	0.000	0.638
H11-N20	0.011	0.039	0.008	-0.007	0.001	0.875
C14-C15	0.319	-0.870	0.115	-0.449	-0.333	3.881
C15-N18	0.311	-0.327	0.415	-0.913	-0.497	2.197
C16-C17	0.319	-0.871	0.114	-0.446	-0.332	3.904
C16-N23	0.329	0.329	0.308	-0.873	-0.529	2.716
C17-N21	0.311	0.311	0.427	-0.925	-0.498	2.167
N18-N19	0.390	-0.802	0.221	-0.643	-0.422	2.904
N19-N20	0.424	-0.963	0.242	-0.726	-0.483	2.991
N21-N22	0.387	-0.789	0.219	-0.636	-0.417	2.898
N22-N23	0.423	-0.959	0.242	-0.724	-0.482	2.988
O52-H57	0.011	0.045	0.010	-0.008	0.001	0.871
RCPs						
RCP1	0.014	0.077	0.016	-0.014	0.002	0.849
RCP2	0.009	0.043	0.008	-0.006	0.002	0.762
RCP3	0.003	0.010	0.002	-0.001	0.000	0.697
RCP4	0.008	0.039	0.008	-0.006	0.001	0.790
RCP5	0.056	0.507	0.111	-0.095	0.015	0.859
RCP6	0.056	0.506	0.111	-0.095	0.015	0.859
RCP7	0.000	0.000	0.000	-0.000	0.000	0.370
RCP8	0.021	0.166	0.032	-0.024	0.008	0.731
RCP9	0.021	0.167	0.032	-0.024	0.008	0.731

Table S3. Topological parameters of some selected BCPs and RCPs related to TS-1, via the QTAIM approach at M06/6-311G** calculated wave function of electron density. Note that numbering of atoms is in accordance with Fig. 4

	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b	$\lvert V_b\rvert/G_b$
BCPs						
C1-C2	0.228	-0.484	0.052	-0.227	-0.174	4.286
C1-C3	0.233	-0.507	0.052	-0.232	-0.179	4.400
C1-C4	0.429	-0.591	0.053	-0.255	-0.201	4.746
C3-C7	0.268	-0.685	0.067	-0.307	-0.239	4.527
C7-C8	0.419	-0.858	0.532	-1.279	-0.747	2.402
C5-O11	0.249	-0.473	0.226	-0.572	-0.345	2.522
C7-O10	0.009	0.035	0.008	-0.007	0.000	0.905
C7-O11	0.010	0.035	0.008	-0.007	0.000	0.905
O10-O11	0.010	0.038	0.009	-0.009	0.0001	0.985
C8-Cu23	0.170	0.371	0.199	-0.306	-0.106	1.534
RCPs						
RCP1	0.009	0.041	0.008	-0.007	0.001	0.839
RCP2	0.009	0.045	0.010	-0.008	0.001	0.877
RCP3	0.009	0.041	0.009	-0.007	0.001	0.838

Table S4. Topological parameters of some selected BCPs and RCPs related to TS-2, via the QTAIM approach at M06/6-311G** calculated wave function of electron density. Note that numbering of atoms is in accordance with Fig. 4

	ρ_b	$\nabla^2\rho_b$	G_b	V_b	H_b	$\lvert V_b\rvert/G_b$
BCPs						
C1-C2	0.247	-0.580	0.053	-0.251	-0.198	4.726
C1-C3	0.247	-0.582	0.053	-0.253	-0.199	4.710
C1-C4	0.238	-0.528	0.055	-0.242	-0.187	4.395
C2-O18	0.247	-0.410	0.243	-0.588	-0.345	2.422
C5-C11	0.264	-0.660	0.067	-0.302	-0.233	4.401
C10-C12	0.405	-0.900	0.484	-1.194	-0.709	2.464
C11-C13	0.406	-0.866	0.494	-1.206	-0.711	2.437
C11-O18	0.022	0.088	0.020	-0.018	0.001	0.923
C12-Cu23	0.120	0.210	0.123	-0.194	-0.071	1.574
C13-Cu22	0.121	0.201	0.122	-0.194	-0.071	1.588
RCPs						
RCP1	0.015	0.086	0.018	-0.014	0.003	0.812