Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

On the Nature of Organic Electron Density Transfer Complexes within the Molecular Electron Density Theory

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1. Study of the formation of the molecular complexes between acenaphtalene and the cyclic anhydride derivatives. Selection of the computational method.

In 1974, Nagy et al. studied the effects of the electron-withdrawing substitution on cyclic anhydrides in the formation of a series of molecular complexes (MCs) with acenaphtalene (**ACE**) (see Chart S1).[1] In that work, experimental thermodynamic data for the formation of four MCs were reported (see Table S1). In order to select the most appropriate computational method in the study of the formation of MCs of this type, a comparative study of the use of the B3LYP,[2] MPWB1K[3,4] and M06-2X[5] DFT functionals, and the 6-31G(d), 6-31G+(d) and 6-311G(d,p) basis sets[6] was performed for the four MCs given in Table S1. Formation of the corresponding MCs was experimentally found to be exothermic by between −2.4 and −4.0 kcal·mol^{-1}. In spite of these low values, in two cases, the formation of the MC was found still exergonic as a consequence of the low unfavourable activation entropy associated to these bimolecular processes (see Table S1).[1]

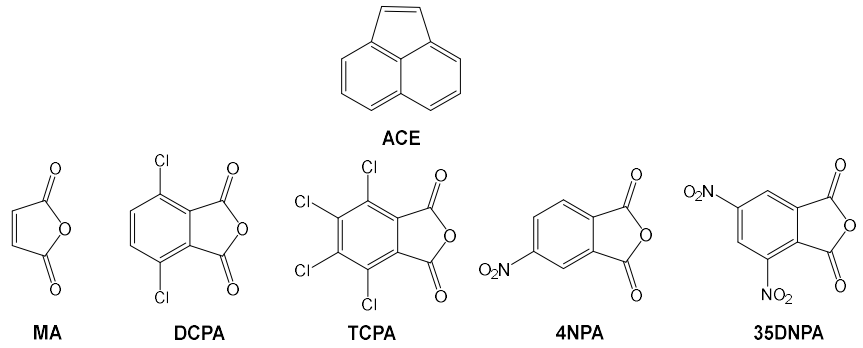

Chart S1. The series of electron-withdrawing substituted cyclic anhydrides used by Nagy et al. in the study of the formation of MCs with **ACE**.

Table S1. Experimental thermodynamic data, in kcal·mol^{-1}, for the formation of four MCs between electron-withdrawing substituted cyclic anhydrides and **ACE**, at 20 ºC in dichloroethane.[1]

	ΔH	-TΔS	ΔG
ACE:DCPA	-2.4 ± 0.4	2.5 ± 0.4	+0.13 ± 0.05
ACE:TCPA	-3.6 ± 0.5	3.2 ± 0.5	-0.43 ± 0.03
ACE:35DNPA	-4.0 ± 0.4	3.5 ± 0.4	-0.53 ± 0.04
ACE:MA	+0.5 ± 0.1	0.6 ± 0.3	+0.10 ± 0.03

The average errors and standard deviations in enthalpies, entropies and Gibbs free energies are given in Table S2. The computed average errors for the formation enthalpy of the **ACE:MA**, **ACE:DCPA**, **ACE:TCPA** and **ACE:35DNPA** MCs using the 6-31G(d) basis set are: 2.3 kcal·mol^{-1} (B3LYP), −3.3 kcal·mol^{-1} (MPWB1K) and −10.0 kcal·mol^{-1} (M06-2X). Consequently, while B3LYP underestimates the enthalpy of formation, MPWB1K and M06-2X overestimate it. A similar trend was observed in the study of the kinetics of polar cycloaddition reactions.[7]

A comparison of the computed entropies of formation, between −20.1 and −45.1 a.u., with that experimentally reported by Nagy et al., −10.9 a.u., shows that the three functionals present high inconsistencies (see Table S2). As a consequence, while the B3LYP and MPWB1K functionals give the formation of these MCs endergonic by between 5.8 and 8.0 kcal·mol^{-1}, the M06-2X functional gives Gibbs free energies of formation by between −4.3 and 4.4 kcal·mol^{-1}.

On the other hand, when the B3LYP and MPWB1K functionals were used together with the larger 6-311G(d,p) basis set, the enthalpy and Gibbs free energies of formation varied only by between −2.3 and 1.9 kcal·mol^{-1} (see Table S2). Finally, when the MPWB1K functional was used together with the 6-31+G(d) basis set, the enthalpy and Gibbs free energies of formation varied by between −0.7 and 2.2 kcal·mol^{-1}. Only the formation enthalpies and Gibbs free energies of **ACE:MA** decreased by ca. 7 kcal·mol^{-1}. Note that this reduction of the^{o} stabilisation of the MC can be associated with the decrease of the Basis Set Superposition Error that appears with the use of the standard 6-3G(d) basis set. Considering that a huge error is introduced in entropies and, thus, in Gibbs free energies as well, the selection was mainly based on enthalpies. Note that although the M062X functional gives the most accurate Gibbs free energies of formation, this is only a fortuity because the high errors in enthalpies and entropies compensate each other. Thus, the MPWB1K and B3LYP functionals yield the lower deviations in the enthalpies of formation with respect to the experimental results. The B3LYP/6-311G(d,p) method affords the most accurate enthalpies; however, it fails giving the **ACE:DCPA** MC as the most stable one. On the other hand, the B3LYP/6-31G(d) method is, on average, 1.0 kcal·mol^{-1} more accurate than the MPWB1K/6-31G(d) method, but gives a higher standard deviation, i.e. 1.9 vs 1.1 kcal·mol^{-1}. A low standard deviation is desirable to maintain the relative trends within the considered series of MCs. Similarly, the MPWB1K/6-31+G(d) method is, on average, 2.0 kcal·mol^{-1} more accurate than the

MPWB1K/6-31G(d) method, but gives a higher standard deviation, i.e. 3.9 vs 1.1 kcal·mol^{-1}. Consequently, and taking into account, moreover, that experimental enthalpies of formation have negative values, the MPWB1K/6-31G(d) method was selected as the most appropriate one for the present study.

Table S2. Average errors between experimental and computed thermodynamic data, at 20 ºC in dichloroethane, for the formation of the **ACE:MA**, **ACE:DCPA**, **ACE:TCPA** and **ACE:35DNPA** MCs, and standard deviations in the enthalpy of formation errors.

	ΔΔH	ΔΔS	ΔΔG	s
B3LYP/6-31G(d)	2.3	-26.5	7.8	1.9
MPWB1K/6-31G(d)	-3.3	-40.9	6.3	1.1
M06-2X/6-31G(d)	-10.0	-39.9	-0.6	1.9
B3LYP/6-311G(d,p)	2.2	-23.9	7.0	1.7
MPWB1K/6-31+G(d)	-1.3	-41.9	8.8	3.8
MPWB1K/6-311G(d,p)	-4.7	-40.0	4.8	0.9

Then, the formation of the MCs between **ACE** and the five cyclic anhydride derivatives given in Chart S1, **MA**, **DCPA**, **TCPA**, **4NPA** and **35DNPA** was studied. The MPWB1K/6-31G(d) thermodynamic data and the values of the global electron density transfer[8] (GEDT) computed at the five MCs are given in Table S3. Formation of the five MCs is exothermic by between −2.4 kcal·mol^{-1} (**ACE:MA**) and −9.0 kcal·mol^{-1} (**ACE:35DNPA**); this trend is similar to that observed in the increase of the electrophilicity ω index[9] within this short series of electrophilic species (see Table S4). Thus, the higher the electrophilic character of the cyclic anhydride derivatives, the more stabilised the MCs. Note that the formation of the five MCs is endergonic because of the high computed negative entropy of formation.

Table S3. MPWB1K/6-31G(d) computed thermodynamic data at 20 ºC in dichloroethane, and GEDT in vacuum, in the formation of the MCs between **ACE** and the cyclic anhydride derivatives.

	ΔH	ΔS	ΔG	GEDT
ACE:MA	-2.4	-35.9	8.2	0.015
ACE:DCPA	-4.9	-39.1	6.0	0.013
ACE:TCPA	-6.6	-42.8	6.0	0.012
ACE:4NPA	-6.4	-41.5	5.7	0.024
ACE:35DNPA	-9.0	-45.1	4.3	0.039

Table S4. MPWB1K/6-31G(d) global electronic chemical potential, μ, chemical hardness, η, electrophilicity, ω, and nucleophilicity, *N*, in eV, of the molecules involved in the formation of the five MCs between **ACE** and the cyclic anhydride derivatives.

	μ	η	ω	*N*
35NPA	-6.79	6.79	3.40	0.04
4NPA	-6.28	6.98	2.82	0.46
TCPA	-5.61	6.32	2.49	1.45
DCPA	-5.36	6.40	2.24	1.67
MA	-5.95	7.46	2.37	0.55
ACE	-3.97	5.64	1.40	3.44

The geometries of the five MCs are given in Figure S1. In the five MCs, the cyclic anhydride is found in a parallel stacking conformation with respect to the molecular plain of **ACE** at a distance between 3.5 Å (**ACE:DCPA**) and 3.1 Å (**ACE:MA**). For the series of the four phthalic anhydride derivatives, the more electrophilic the phthalic anhydride, the shorter the distance.

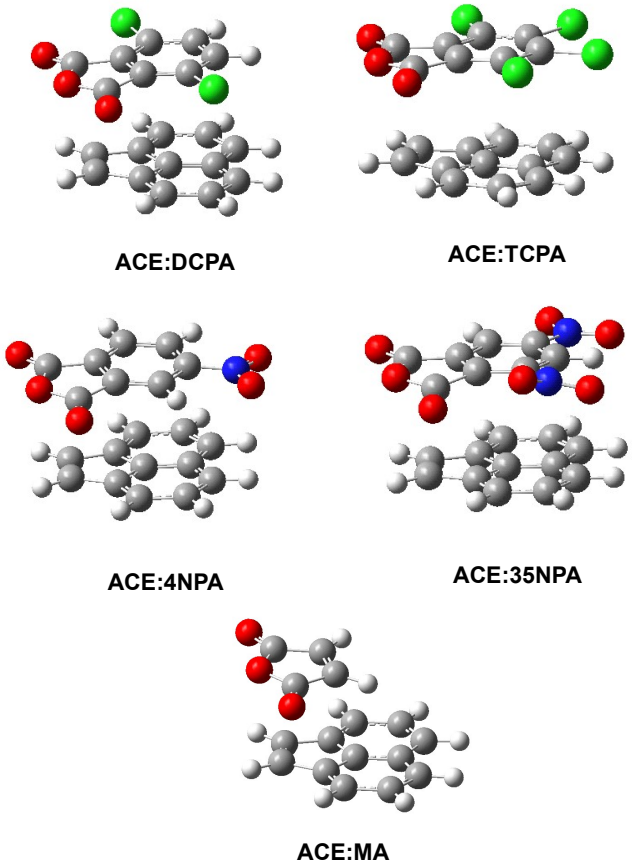

Figure S1. MPWB1K/6-31G(d) geometries in vacuum of the MCs between **ACE** and the cyclic anhydride derivatives.

The GEDT in these MCs, which takes place from **ACE**, acting as nucleophile, to the electrophilic cyclic anhydride derivatives, is: 0.015 e at **ACE:MA**, 0.013 e at **ACE:DCPA**, 0.012 e at **ACE:TCPA**, 0.024 e at **ACE:4NPA** and 0.039 e at **ACE:35DNPA** (see Table S2). These values indicate that these MCs have a very low polar character, in spite of the strong nucleophilic character of **ACE** and the strong electrophilic character of the cyclic anhydride derivatives. This result can be a consequence of the high aromatic character of **ACE**.

Finally, the dependence of the GEDT with the computational level of theory was analysed by evaluating the GEDT at the most polar **ACE:35DNPA** MC at the different computational levels selected previously for the evaluation of the thermodynamic data (see Table S5). As can be observed, the values of the GEDT at **ACE:35DNPA** are found in a narrow range, from 0.02 to 0.04 e, indicating the low dependence of the GEDT with the computational level. This dependency is even lower when only changes in the basis set are considered; e.g. 0.03 e (MPWB1K/6-31+G(d) and 0.04 e (MPWB1K/6-31G(d)). Note that the enthalpy of formation of this MC varies in a wider range, from −0.9 (B3LYP/6-31G(d)) to −16.7 (M06-2X/6-31G(d)) kcal·mol^{-1} (see Tables S6 and S8).

Table S5. Computed GEDT values, in e, at different computational levels of theory for the most polar **ACE:35DNPA** MC.

	GEDT
B3LYP/6-31G(d)	0.023
MPWB1K/6-31G(d)	0.039
M06-2X/6-31G(d)	0.041
B3LYP/6-311G(d,p)	0.017
MPWB1K/6-31+G(d)	0.032
MPWB1K/6-311G(d,p)	0.035

In accordance with the proposed definition of an electron density transfer complex (EDTC), the low GEDT values computed at these MCs categorised by Nagy et al. as “charge-transfer complexes”, together their low thermodynamic stability, do not permit their classification as EDTCs.

References

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*2. Analysis of the vdW interactions in the **TEE:BZ** and **TCE-BZ4O** MCs*

Figure S2 shows the changes in the topological analysis of the electron density associated with NCIs when the equilibrium distance between the two interacting frameworks in **TEE:BZ**, 3.46 Å, is shortened to 3.20 (**TEE:BZ** (3.20)) and 2.96 (**TEE:BZ** (2.96)) Å. Ongoing from 3.46 to 2.96 Å, the green colour of the NCI surface shifts towards blue and red (the highest electron density overlaps), which confirms the expected increase of the electron density overlap with the decrease of the distance. As the GEDT in **TEE:BZ** is null and both constrained structures are destabilised by 0.8 (**TEE:BZ** (3.20)) and 4.8 (**TEE:BZ** (2.96)) kcal·mol^{-1}, it can be considered that vdW radii in the twelve studied MCs are overcome at distances below ca. 3.20 Å.

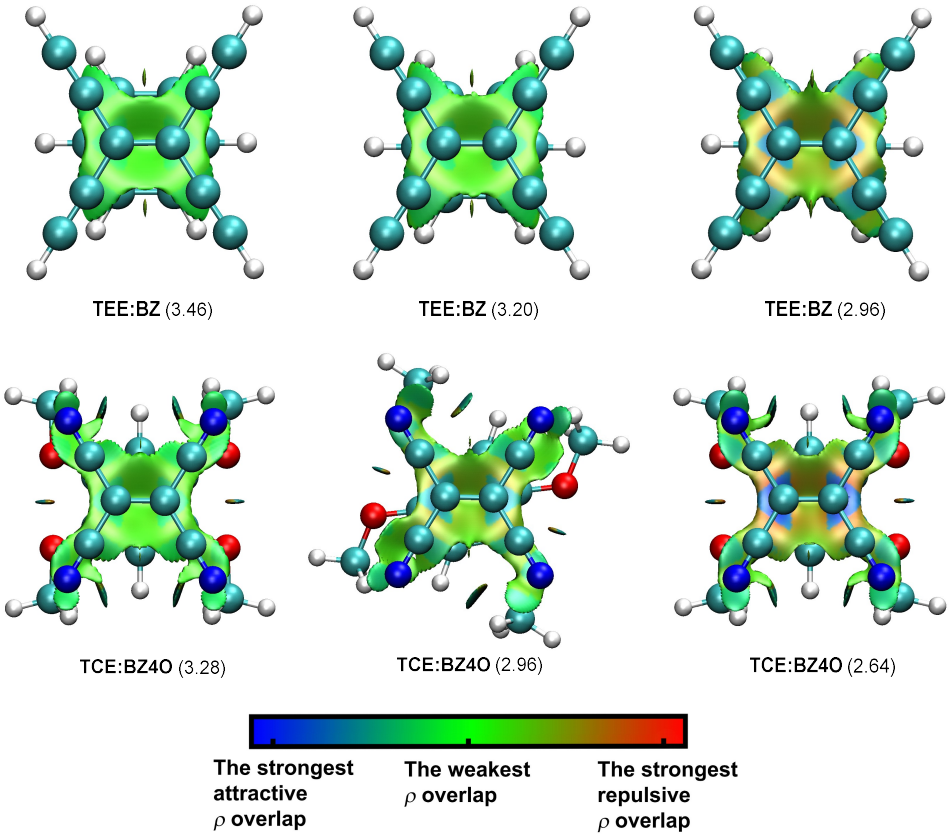

Figure S2. NCI gradient isosurfaces of **TEE-BZ** and structures **TEE-BZ** (3.20) and **TEE-BZ** (2.96), and those of **TCE-BZ4O** and **TCE-BZ4O** (3.28) and **TCE-BZ4O** (2-64). Surfaces are coloured in the [−0.025, 0.025] a.u. range of sign(λ_2)ρ (isosurfaces = 0.5 a.u.).

When the intermolecular distance in **TCE:BZ4O**, 2.96 Å, is enlarged to 3.28 Å in **TCE:BZ4O** (3.28) and shortened to 2.64 Å in **TCE:BZ4O** (2.64), the same trend is observed (see Figure S2). Ongoing from **TCE:BZ4O** (3.28) to **TCE:BZ4O** (2.64), there

is a gradual separation of the practically homogeneous green colour of the NCI surface in **TCE:BZ4O** (3.28) towards blue and red, indicating that the shorter the distance, the higher the electron density overlap. According to the previous analysis, we can suppose that vdW repulsions exist in the three considered structures of **TCE:BZ4O**; however, it is interesting to note that at equivalent intermolecular distances and, therefore, NCI surfaces and vdW interactions, the structures of **TCE:BZ4O** are more stabilised than those of **TEE:BZ** due to the GEDT. For instance, both **TCE:BZ4O** (3.28) and **TCE:BZ4O** (2.64) are destabilised by 2.4 and 2.7 kcal·mol^{-1} with respect to **TCE:BZO4** (2.96); however, while **TCE:BZ4O** (2.96), which is at the equilibrium distance, is more stable than **TCE:BZ4O** (3.28 Å), the equivalent structure of **TEE:BZ** at 3.28 Å should be more destabilised with respect to the corresponding structure at 3.20 Å. These results emphasize the greater weight of the GEDT in the stabilisation of EDTCs. At distances below 3.00 Å, vdW repulsions begin to overcome the GEDT, while at distances above 3.00 Å, the GEDT loses somewhat effectivity, thus constituting unfavourable situations. Note that the GEDT depends on the distance.

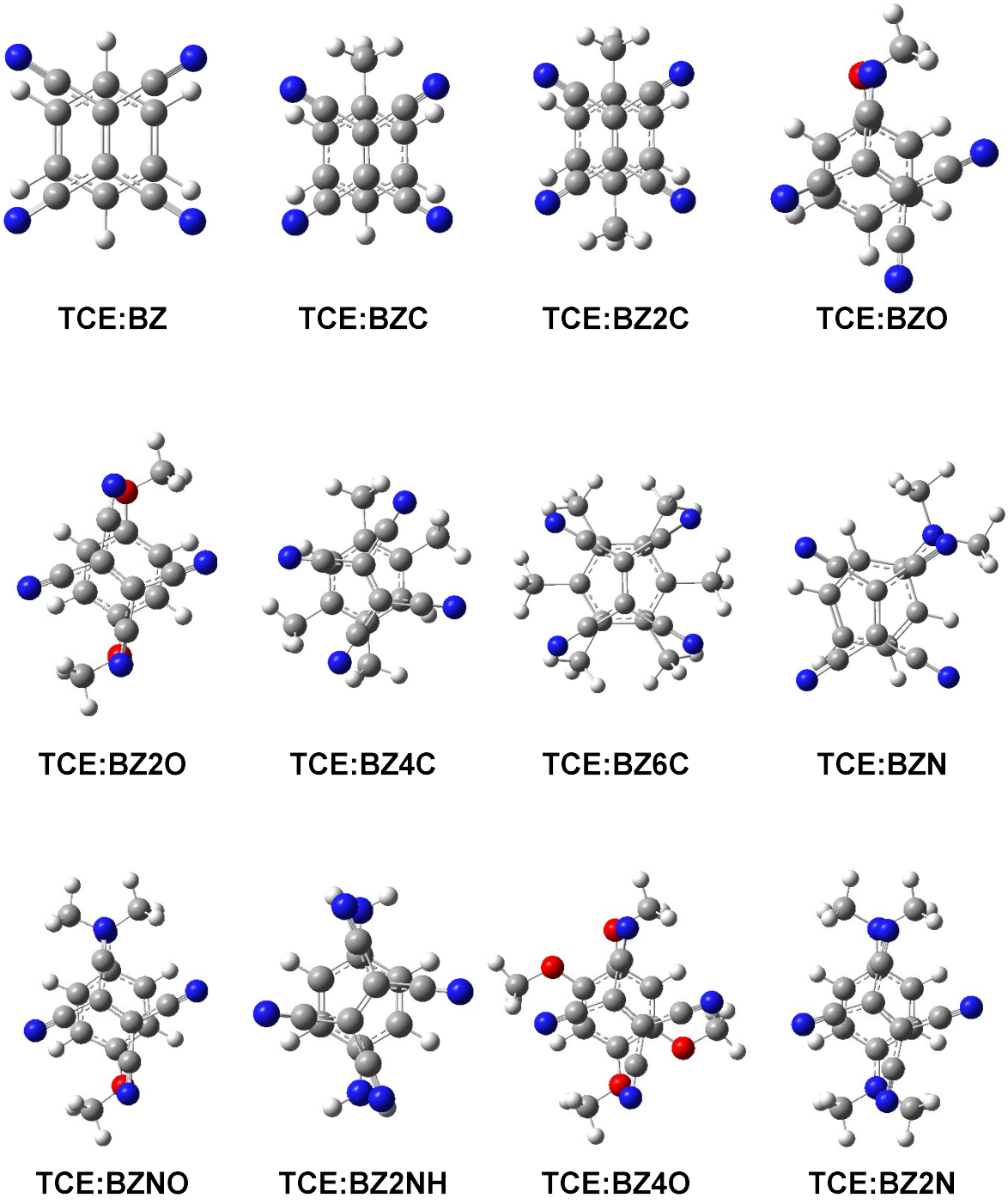

Figure S3. Top view of the MPWB1K/6-31G(d) geometries of the MCs formed between **TCE** and the twelve selected benzene derivatives.

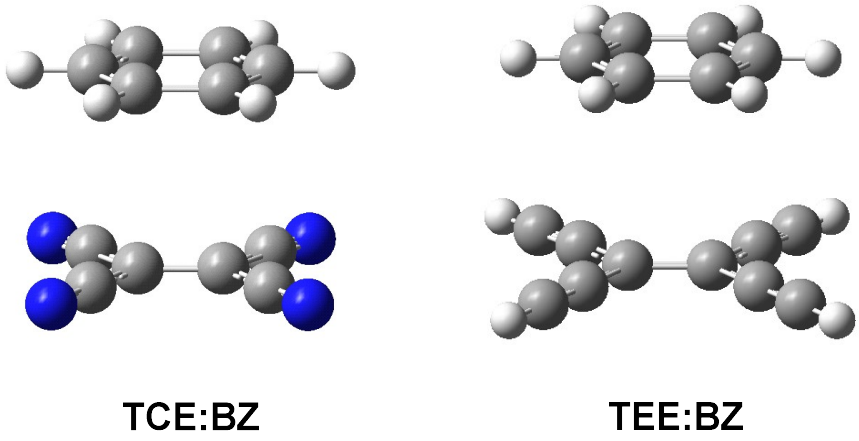

Figure S4. MPWB1K/6-31G(d) geometries of the isoelectronic **TCE:BZ** and **TEE:BZ** MCs.

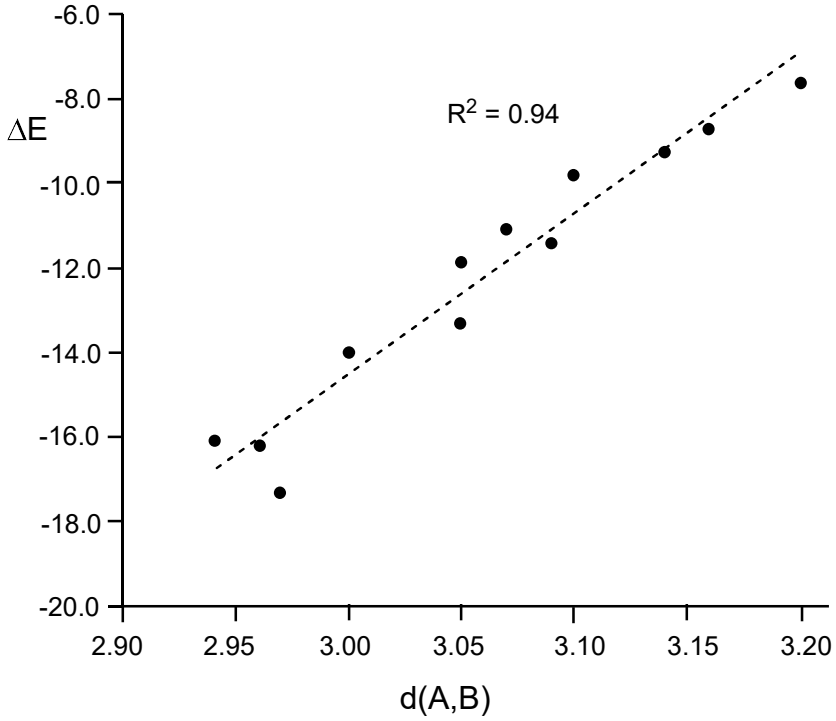

Figure S5. Plot of the MPWB1K/6-31G(d) energy of formation in vacuum, ΔE in kcal·mol^{-1}, vs the distance between the two species, d(A,B) in angstroms, Å, involved in the MCs formed between **TCE** and the twelve benzene derivatives.

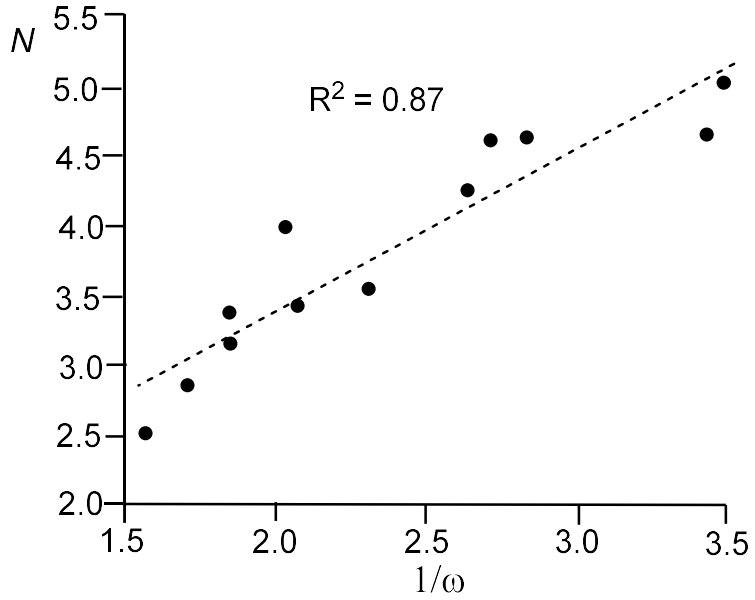

Figure S6. Plot of the nucleophilicity *N* index, in eV, vs the inverse of the electrophilicity ω index, in eV, for the twelve benzene derivatives.

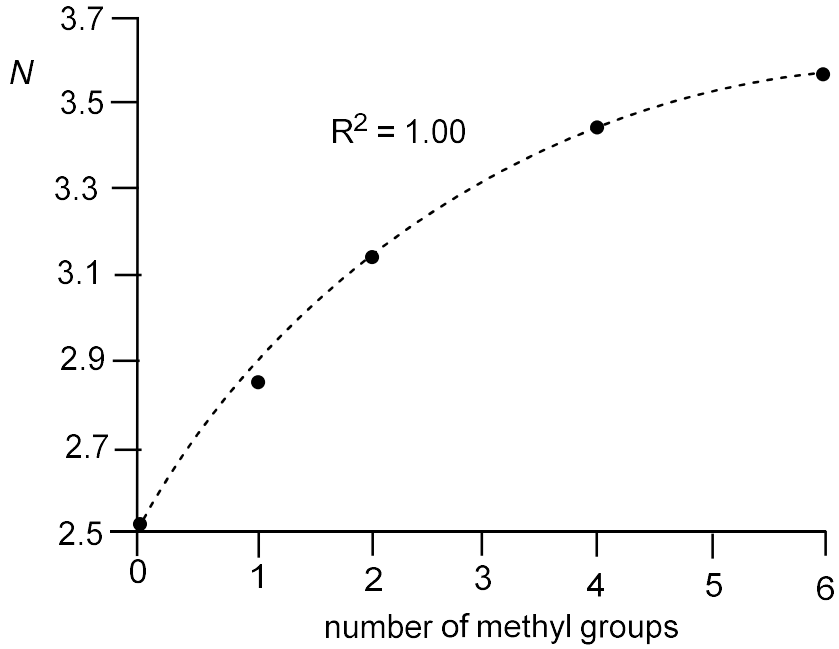

Figure S7. Plot of the nucleophilicity *N* index, in eV, with respect to the number of methyl substituents in the **BZ**, **BZC**, **BZ2C**, **BZ6C** and **BZ4C** benzene derivative series.

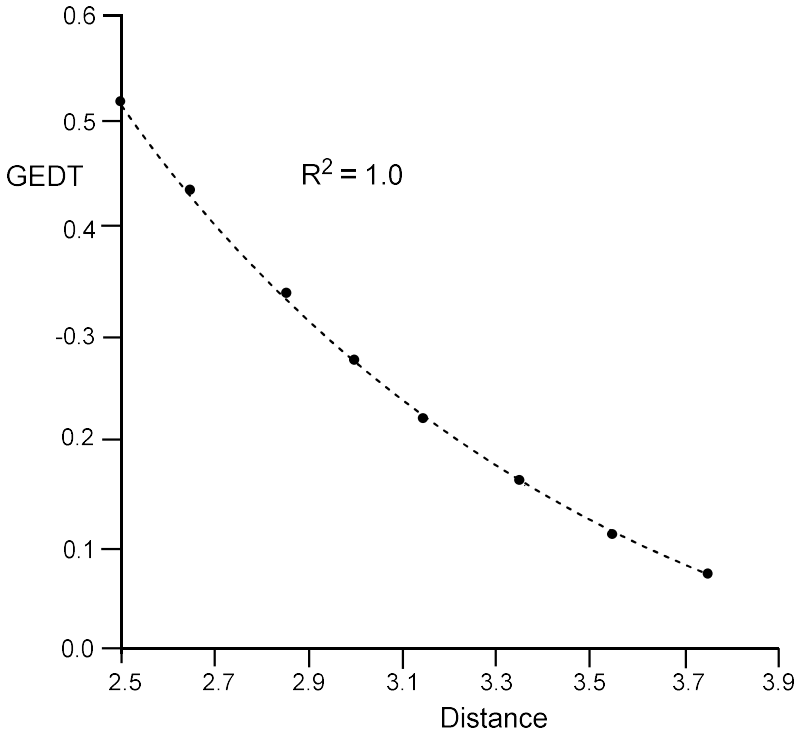

Figure S8. Plot of the GEDT, in average number of electrons, e, with respect to the distance, in angstroms, Å, of the two fragments of the **TCE:BZ4O** EDTC.

Table S6. B3LYP/6-31G(d) computed enthalpies (H), entropies (S) and Gibbs free energies (G), in atomic units, a.u., and the relative ones, ΔH and ΔG in kcal·mol^{-1}, and ΔS in cal·mol^{-1}·K^{-1}, at 20 ºC in dichloroethane, for the structures involved in the formation of the four MCs between **ACE** and cyclic anhydride derivatives for which experimental thermodynamic data was reported,[1] together with the average errors between the computed and the experimental thermodynamic data.

	H	S	G	ΔH	ΔS	ΔG	ΔΔH	ΔΔS	ΔΔG
ACE	-461.923673	85.534	-461.963631						
MA	-379.236359	73.742	-379.270809						
DCPA	-1452.045231	99.108	-1452.091531						
TCPA	-2371.231770	112.404	-2371.284281						
35DNPA	-941.817187	110.184	-941.868661						
ACE:MA	-841.159954	133.109	-841.222137	0.0	-26.2	7.7	-0.5	-26.8	7.6
ACE:DCPA	-1913.968499	158.755	-1914.042663	0.3	-25.9	7.8	2.7	-25.9	7.7
ACE:TCPA	-2833.155198	173.151	-2833.236088	0.2	-24.8	7.4	3.8	-24.8	7.8
ACE:35DNPA	-1403.742336	166.982	-1403.820344	-0.9	-28.7	7.5	3.1	-28.7	8.0
Average							2.3	-26.5	7.8

Table S7. MPWB1K/6-31G(d) computed enthalpies (H), entropies (S) and Gibbs free energies (G), in atomic units, a.u., and the relative ones, ΔH and ΔG in kcal·mol^{-1}, and ΔS in cal·mol^{-1}·K^{-1}, at 20 ºC in dichloroethane, for the structures involved in the formation of the four MCs between **ACE** and cyclic anhydride derivatives for which experimental thermodynamic data was reported,[1] together with the average errors between the computed and the experimental thermodynamic data.

	H	S	G	ΔH	ΔS	ΔG	ΔΔH	ΔΔS	ΔΔG
ACE	-461.693453	85.048	-461.733184						
MA	-379.063773	73.191	-379.097965						
DCPA	-1451.921820	98.349	-1451.966837						
TCPA	-2371.220625	110.968	-2371.272465						
35DNPA	-941.415727	113.311	-941.468662						
ACE:MA	-1403.123460	153.254	-1403.195055	-2.4	-35.9	8.2	-2.9	-36.5	8.1
ACE:DCPA	-2832.924534	153.236	-2832.996120	-4.9	-39.1	6.0	-2.5	-39.0	5.8
ACE:TCPA	-1913.623082	144.342	-1913.690513	-6.6	-42.8	6.0	-3.0	-42.8	6.4
ACE:35DNPA	-840.760981	122.343	-840.818135	-9.0	-45.1	4.3	-5.0	-45.1	4.8
Average							-3.3	-40.9	6.3

Table S8. M06-2X/6-31G(d) computed enthalpies (H), entropies (S) and Gibbs free energies (G), in atomic units, a.u., and the relative ones, ΔH and ΔG in kcal·mol^{-1}, and ΔS in cal·mol^{-1}·K^{-1}, at 20 ºC in dichloroethane, for the structures involved in the formation of the four MCs between **ACE** and cyclic anhydride derivatives for which experimental thermodynamic data was reported,[1] together with the average errors between the computed and the experimental thermodynamic data.

	H	S	G	ΔH	ΔS	ΔG	ΔΔH	ΔΔS	ΔΔG
ACE	-461.723052	85.489	-461.762989						
MA	-379.089390	73.616	-379.123781						
DCPA	-1451.785801	98.926	-1451.832016						
TCPA	-2370.924510	112.083	-2370.976871						
35DNPA	-941.459535	109.501	-941.510690						
ACE:MA	-840.824173	118.538	-840.879550	-7.4	-40.6	4.5	-7.9	-41.2	4.4
ACE:DCPA	-1913.527684	146.073	-1913.595924	-11.8	-38.3	-0.6	-9.4	-38.3	-0.7
ACE:TCPA	-2832.669802	157.179	-2832.743231	-14.0	-40.4	-2.1	-10.4	-40.4	-1.7
ACE:35DNPA	-1403.208820	155.384	-1403.281410	-16.5	-39.6	-4.9	-12.5	-39.6	-4.3
Average							-10.0	-39.9	-0.6

Table S9. B3LYP/6-311G(d,p) computed enthalpies (H), entropies (S) and Gibbs free energies (G), in atomic units, a.u., and the relative ones, ΔH and ΔG in kcal·mol^{-1}, and ΔS in cal·mol^{-1}·K^{-1}, at 20 ºC in dichloroethane, for the structures involved in the formation of the four MCs between **ACE** and cyclic anhydride derivatives for which experimental thermodynamic data was reported,[1] together with the average errors between the computed and the experimental thermodynamic data.

	H	S	G	ΔH	ΔS	ΔG	ΔΔH	ΔΔS	ΔΔG
ACE	-462.030856	85.766	-462.070923						
MA	-379.340716	73.750	-379.375169						
DCPA	-1452.233439	99.226	-1452.279794						
TCPA	-2371.470962	112.687	-2371.523605						
35DNPA	-942.065269	115.008	-942.118997						
ACE:MA	-841.370826	139.994	-841.436226	0.5	-19.5	6.2	0.0	-20.1	6.1
ACE:DCPA	-1914.265068	163.804	-1914.341592	-0.5	-21.2	5.7	1.9	-21.2	5.6
ACE:TCPA	-2833.502444	177.105	-2833.585181	-0.4	-21.3	5.9	3.2	-21.3	6.3
ACE:35DNPA	-1404.096498	167.823	-1404.174899	-0.2	-33.0	9.4	3.8	-32.9	10.0
Average							2.2	-23.9	7.0

Table S10. MPWB1K/6-31+G(d) computed enthalpies (H), entropies (S) and Gibbs free energies (G), in atomic units, a.u., and the relative ones, ΔH and ΔG in kcal·mol^{-1}, and ΔS in cal·mol^{-1}·K^{-1}, at 20 ºC in dichloroethane, for the structures involved in the formation of the four MCs between **ACE** and cyclic anhydride derivatives for which experimental thermodynamic data was reported,[1] together with the average errors between the computed and the experimental thermodynamic data.

	H	S	G	ΔH	ΔS	ΔG	ΔΔH	ΔΔS	ΔΔG
ACE	-461.705777	85.217	-461.745587						
MA	-379.086865	73.353	-379.121133						
DCPA	-1451.936418	100.034	-1451.983151						
TCPA	-2371.235993	111.384	-2371.288027						
35DNPA	-941.446453	113.895	-941.499661						
ACE:MA	-840.784739	124.789	-840.843036	5.0	-33.8	14.9	4.5	-34.4	14.8
ACE:DCPA	-1913.651043	138.468	-1913.715731	-5.6	-46.8	8.2	-3.2	-46.8	8.0
ACE:TCPA	-2832.951624	154.605	-2833.023851	-6.2	-42.0	6.1	-2.6	-42.0	6.6
ACE:35DNPA	-1403.164597	154.782	-1403.236905	-7.8	-44.3	5.2	-3.8	-44.3	5.8
Average							-1.3	-41.9	8.8

Table S11. MPWB1K/6-311G(d,p) computed enthalpies (H), entropies (S) and Gibbs free energies (G), in atomic units, a.u., and the relative ones, ΔH and ΔG in kcal·mol^{-1}, and ΔS in cal·mol^{-1}·K^{-1}, at 20 ºC in dichloroethane, for the structures involved in the formation of the four MCs between **ACE** and cyclic anhydride derivatives for which experimental thermodynamic data was reported,[1] together with the average errors between the computed and the experimental thermodynamic data.

	H	S	G	ΔH	ΔS	ΔG	ΔΔH	ΔΔS	ΔΔG
ACE	-461.789268	85.181	-461.829061						
MA	-379.169522	73.299	-379.203765						
DCPA	-1452.09504	98.300	-1452.14096						
TCPA	-2371.4431	111.08	-2371.495						
35DNPA	-941.645992	113.584	-941.699054						
ACE:MA	-840.963994	125.436	-841.022593	-3.3	-33.0	6.4	-3.8	-33.6	6.3
ACE:DCPA	-1913.89485	144.049	-1913.96214	-6.6	-39.4	4.9	-4.2	-39.4	4.8
ACE:TCPA	-2833.24599	154.421	-2833.31813	-8.5	-41.8	3.7	-4.9	-41.8	4.2
ACE:35DNPA	-1403.45075	153.781	-1403.52259	-9.7	-45.0	3.5	-5.7	-45.0	4.0
Average							-4.7	-40.0	4.8

MPWB1K/6-31G(d) Cartesian coordinates and electronic energies of the **TEE:BZ** MC and the twelve MCs between **TCE** and the benzene derivatives.

TEE:BZ
E(RmPW+HF-B95) = -615.079211693 AU

C	-1.35576700	0.00276300	0.68299400
C	-1.35881300	0.00167800	-0.67826800
C	-1.37267200	-1.20977900	-1.41621800
C	-1.36723300	1.21203300	-1.41809800
C	-1.36647400	-1.20757100	1.42285600
C	-1.36131400	1.21423100	1.42103500
C	2.10152200	1.19428800	0.68951800
C	2.09716600	1.19589900	-0.69414100
C	2.09477200	-0.00186700	-1.38767000
C	2.09340300	-1.20122000	-0.69691400
C	2.09744200	-1.20281000	0.68675800
C	2.10323100	-0.00507200	1.38026500
H	2.08988800	2.12806700	1.23084400
H	2.08221600	2.13094800	-1.23319100
H	2.08013900	-0.00058200	-2.46718500
H	2.07542700	-2.13496600	-1.23813000
H	2.08278600	-2.13782500	1.22588300
H	2.09498400	-0.00631800	2.45984700
C	-1.38689600	2.21402800	-2.07750500
H	-1.40690600	3.10789600	-2.64908100
C	-1.37863800	2.21710300	2.07917200
H	-1.39650200	3.11155600	2.64990600
C	-1.39707800	-2.21251600	-2.07434000
H	-1.42020200	-3.10679800	-2.64514800
C	-1.38808100	-2.20941200	2.08243600
H	-1.40925900	-3.10263700	2.65497400

TCE:BZ
E(RmPW+HF-B95) = -679.434812645 AU

C	1.24830000	-0.00054400	-0.67528400
C	1.24801700	0.00104500	0.67598500
C	1.26544000	-1.21366100	1.41829000
N	1.29886000	-2.18543300	2.03225000
C	1.26519800	1.21741400	1.41554700
N	1.29836000	2.19052400	2.02739800
C	1.26698200	-1.21696100	-1.41473700
N	1.30153000	-2.19010400	-2.02645800
C	1.26587500	1.21413400	-1.41761500
N	1.29931600	2.18591100	-2.03156500
C	-1.94659400	1.20086100	-0.69298800
C	-1.94677500	1.20116300	0.69125900
C	-1.94625500	-0.00005500	1.38379500
C	-1.94703500	-1.20156300	0.69183200
C	-1.94672500	-1.20186700	-0.69242800
C	-1.94588800	-0.00066200	-1.38497300
H	-1.94241900	2.13485000	-1.23403900

H	-1.94251100	2.13537700	1.23191900
H	-1.95006200	0.00019300	2.46365700
H	-1.94292500	-2.13553900	1.23290100
H	-1.94240400	-2.13608600	-1.23308100
H	-1.94937600	-0.00089800	-2.46483400

TCE:BZC

E(RmPW+HF-B95) = -718.730173310 AU

C	-0.55269200	-1.32043100	0.00791100
C	-1.57306300	-0.43401500	-0.00044300
C	-2.14246300	0.02614100	-1.22130200
N	-2.62679500	0.38800200	-2.19958400
C	-2.14826000	0.04269300	1.21130600
N	-2.63721300	0.41789100	2.18223800
C	0.00373400	-1.83049300	-1.19957400
N	0.46627300	-2.26811700	-2.15740800
C	-0.00221000	-1.81484900	1.22459000
N	0.45540200	-2.24039100	2.19019900
C	1.52191700	1.03269400	1.18983500
C	0.51507600	1.98045700	1.19069000
C	0.00138400	2.45011000	-0.00801000
C	0.51195400	1.97123300	-1.20442800
C	1.51867100	1.02332900	-1.19901700
C	2.03800400	0.53664500	-0.00338000
H	1.90632100	0.65746400	2.12756400
H	0.12079900	2.34444300	2.12735400
H	0.11510000	2.32790100	-2.14282600
H	1.90035700	0.64061500	-2.13483900
C	3.12428800	-0.49163900	-0.00074400
H	3.06653400	-1.12963300	-0.88001700
H	4.10641800	-0.01963000	-0.00466900
H	3.06979200	-1.12164100	0.88450500
H	-0.78703000	3.18753700	-0.00979700

TCE:BZ2C

E(RmPW+HF-B95) = -758.025373195 AU

C	0.67424600	-1.45833800	0.00395700
C	-0.67815900	-1.45633700	0.00130400
C	-1.42197900	-1.47730700	-1.21264300
N	-2.04830400	-1.50977800	-2.17689600
C	-1.42687900	-1.47137700	1.21231800
N	-2.05731900	-1.49886400	2.17404500
C	1.42271400	-1.48179300	-1.20708700
N	2.05258700	-1.51680600	-2.16893600
C	1.41808500	-1.47631400	1.21793000
N	2.04436500	-1.50707400	2.18226800
C	0.69285400	1.65636300	1.18804700
C	-0.68824100	1.65725600	1.18807200
C	-1.40704600	1.64459500	-0.00295800
C	-0.68831200	1.65140200	-1.19400300
C	0.69285900	1.65047200	-1.19402100

C	1.41162300	1.64275200	-0.00301200
H	1.22611400	1.64048900	2.12793100
H	-1.22152600	1.64185800	2.12795100
H	-1.22160600	1.63139000	-2.13378600
H	1.22608700	1.62993400	-2.13383100
C	-2.90219400	1.62348000	-0.00265800
H	-3.30773900	2.63497600	-0.00122800
H	-3.28972700	1.11876300	-0.88515600
H	-3.28919500	1.11651800	0.87881200
C	2.90674400	1.62059300	-0.00287000
H	3.29388900	1.11547700	-0.88529200
H	3.31282200	2.63188000	-0.00167300
H	3.29369500	1.11368600	0.87865200

TCE:BZO

E(RmPW+HF-B95) = -793.907939586 AU

C	1.55722800	0.82081300	-0.40257300
C	0.92838300	0.99767600	0.78201500
C	1.43355200	0.41676200	1.97958000
N	1.84640200	-0.03043500	2.95533300
C	-0.23625700	1.80882000	0.88540700
N	-1.16485700	2.48053900	0.98353700
C	2.75001900	0.05069800	-0.50286800
N	3.72788500	-0.54736300	-0.59724400
C	1.07211400	1.43683400	-1.59085000
N	0.69684100	1.94481800	-2.55204100
C	-0.30457000	-1.48935300	-1.67542500
C	-1.41314300	-0.78120800	-1.23595700
C	-1.77074100	-0.83758400	0.10461700
C	-0.99595600	-1.58248400	0.99449100
C	0.10561600	-2.27814900	0.54202900
C	0.46061200	-2.23845000	-0.79861700
H	-0.04053100	-1.44627400	-2.72165000
H	-1.98832600	-0.20251000	-1.93959000
H	-1.29036400	-1.60579300	2.03228200
H	0.69377600	-2.85109200	1.24259200
O	-2.82290200	-0.20307300	0.63589200
C	-3.63477700	0.55871500	-0.21728000
H	-4.41116200	0.98255500	0.40737400
H	-3.07101400	1.36536800	-0.68266700
H	-4.08712200	-0.06574300	-0.98756000
H	1.32158400	-2.78337200	-1.15243700

TCE:BZ2O

E(RmPW+HF-B95) = -908.378733060 AU

C	0.38451300	1.63296600	-0.55845200
C	-0.38495200	1.63296200	0.55822400
C	0.20593200	1.66481300	1.85282400
N	0.68304900	1.71006800	2.89853000
C	-1.80450700	1.65898100	0.48083200
N	-2.95346300	1.69797800	0.43232500

C	1.80406000	1.65934600	-0.48103700
N	2.95301000	1.69850000	-0.43250600
C	-0.20638900	1.66449300	-1.85305100
N	-0.68355900	1.70956700	-2.89874100
C	0.41206100	-1.42855200	-1.31232300
C	-0.93889100	-1.43325800	-1.02475600
C	-1.36506400	-1.44023400	0.29805800
C	-0.41164600	-1.42816400	1.31247400
C	0.93930600	-1.43283000	1.02490800
C	1.36547400	-1.44020000	-0.29790100
H	0.75430300	-1.42806000	-2.33565500
H	-1.64663500	-1.42887300	-1.83715400
H	-0.75388400	-1.42738200	2.33580700
H	1.64706000	-1.42805700	1.83729900
O	2.64904800	-1.45003000	-0.68674300
O	-2.64863600	-1.45020200	0.68692300
C	3.63423200	-1.47843400	0.31066700
H	4.58558100	-1.47366700	-0.20657800
H	3.57376900	-0.60096100	0.95237900
H	3.55265000	-2.38196700	0.91533900
C	-3.63386900	-1.47907700	-0.31042700
H	-4.58519400	-1.47419000	0.20686000
H	-3.57351100	-0.60184100	-0.95246900
H	-3.55224400	-2.38282600	-0.91477100

TCE:BZ4C

E(RmPW+HF-B95) = -836.616074493 AU

C	0.41326600	1.64231700	-0.53626300
C	-0.41296400	1.64244700	0.53602400
C	0.10242000	1.67061900	1.86271700
N	0.51188000	1.71749100	2.93655700
C	-1.82586700	1.67661900	0.37767200
N	-2.96983000	1.73346500	0.26576000
C	1.82618200	1.67629700	-0.37797400
N	2.97015900	1.73307200	-0.26617500
C	-0.10214300	1.67034400	-1.86295000
N	-0.51160600	1.71712100	-2.93679300
C	-0.01957900	-1.43836900	-1.36249400
C	-1.22859500	-1.43503700	-0.68657800
C	-1.20962200	-1.45039200	0.71175500
C	0.01933000	-1.43801500	1.36273800
C	1.22834500	-1.43499500	0.68681700
C	1.20937300	-1.45073000	-0.71151000
H	-0.03151600	-1.43897600	-2.44428200
H	0.03126900	-1.43840500	2.44452600
C	-2.48283200	-1.52093800	1.48956900
H	-3.00833000	-2.45455800	1.28702700
H	-2.29569500	-1.46973000	2.55862000
H	-3.16603000	-0.71462500	1.22410700
C	2.48255800	-1.52167000	-1.48933000
H	3.16584100	-0.71532200	-1.22421000
H	3.00798900	-2.45525900	-1.28647900
H	2.29538200	-1.47083800	-2.55839300

C	-2.52305700	-1.43736500	-1.43277900
H	-3.10064100	-2.33682200	-1.21896900
H	-3.14675400	-0.58800900	-1.15431600
H	-2.35702300	-1.39163400	-2.50535100
C	2.52279500	-1.43735300	1.43305100
H	3.09995500	-2.33724100	1.21989000
H	3.14691600	-0.58849200	1.15402300
H	2.35674800	-1.39081600	2.50558600

TCE:BZ6C

E(RmPW+HF-B95) = -915.192060863 AU

C	-0.17786200	0.67616100	1.76534800
C	-0.17441800	-0.67954000	1.76463200
C	1.03487400	-1.41328100	1.90601200
N	2.00287800	-2.01803300	2.05463100
C	-1.39319500	-1.41064200	1.71246000
N	-2.38101900	-2.00095800	1.70289000
C	1.02770100	1.41581100	1.90776200
N	1.99267200	2.02508500	2.05764000
C	-1.40029200	1.40117000	1.71364400
N	-2.39113600	1.98641400	1.70425900
C	-0.57110900	1.21064700	-1.33350300
C	-1.26864500	0.00177400	-1.39386200
C	-0.57204900	-1.20763600	-1.33593800
C	0.82722000	-1.20655500	-1.23564400
C	1.51687800	0.00064900	-1.12139700
C	0.82816700	1.20850800	-1.23374100
C	-1.31476800	-2.50914900	-1.40499500
H	-1.45133900	-2.83609800	-2.43754300
H	-0.78793500	-3.30048000	-0.88068900
H	-2.29794900	-2.43422500	-0.95275400
C	1.60150300	2.49013800	-1.32315400
H	1.82142000	2.91880700	-0.34402500
H	2.55474700	2.32811900	-1.81797800
H	1.06526600	3.23770400	-1.89851400
C	-2.76099300	0.00286700	-1.55532700
H	-3.10317600	-0.86831500	-2.10407800
H	-3.27311700	0.00336100	-0.59058900
H	-3.10166000	0.87469600	-2.10404400
C	2.99920000	-0.00002200	-0.89119400
H	3.56249200	0.00030600	-1.82648000
H	3.30755500	0.87303300	-0.32264800
H	3.30695200	-0.87385700	-0.32354900
C	-1.31350800	2.51248100	-1.39948500
H	-1.45321400	2.84016400	-2.43137800
H	-2.29540100	2.43723500	-0.94439000
H	-0.78493600	3.30333000	-0.87621700
C	1.59976400	-2.48857400	-1.32653300
H	1.06296900	-3.23540900	-1.90231300
H	2.55297600	-2.32665000	-1.82145600
H	1.81978500	-2.91812100	-0.34780600

TCE:BZN

E(RmPW+HF-B95) = -813.334081956 AU

C	0.98045700	0.73481600	-1.03761500
C	1.82083400	-0.29690400	-0.77663700
C	1.54722000	-1.60416700	-1.26687800
N	1.34031100	-2.65728100	-1.68110500
C	3.03633300	-0.10124900	-0.06359900
N	4.03791500	0.04633900	0.48308800
C	-0.20281600	0.56191200	-1.80654200
N	-1.15899900	0.45702100	-2.43914700
C	1.28033100	2.05740800	-0.60353700
N	1.52377000	3.13412300	-0.27994600
C	-0.86997600	0.85890100	1.46714500
C	0.30326000	0.63793200	2.16372800
C	0.85967600	-0.62524300	2.24045900
C	0.20243000	-1.67703700	1.61332300
C	-0.97263400	-1.48004200	0.92212900
C	-1.55320400	-0.20320900	0.84389400
H	-1.27110300	1.85814700	1.42776600
H	0.79363200	1.47642600	2.63501300
H	0.61836300	-2.67287500	1.65505400
H	-1.44455100	-2.32133100	0.44370700
N	-2.71523200	0.00333700	0.17232800
C	-3.23809900	1.33419000	0.04133000
H	-2.53605900	1.99576400	-0.46993500
H	-4.14905500	1.30135400	-0.54389500
H	-3.47563100	1.76842500	1.01319400
C	-3.34851900	-1.09169000	-0.51045000
H	-4.24398200	-0.73114700	-1.00207200
H	-2.69794600	-1.52251700	-1.27218000
H	-3.63837400	-1.87874200	0.18672800
H	1.77859000	-0.79198500	2.77958800

TCE:BZNO

E(RmPW+HF-B95) = -927.805091465 AU

C	-0.00656700	1.58901400	0.70282000
C	0.88449100	1.65398600	-0.32436900
C	0.44823200	1.95588600	-1.64362700
N	0.08937400	2.21714900	-2.70534200
C	2.27890800	1.48991100	-0.11144100
N	3.41378600	1.37513300	0.04500200
C	-1.39463600	1.81183900	0.50679100
N	-2.52501700	1.99193000	0.37699700
C	0.43369400	1.35808600	2.03613100
N	0.79187100	1.18995200	3.11678100
C	-0.56111200	-1.41497700	0.93772700
C	0.80392200	-1.58825400	0.78572300
C	1.38685100	-1.48331300	-0.46590400
C	0.56479000	-1.20798100	-1.56194300
C	-0.79190700	-1.06042900	-1.41931300
C	-1.40445500	-1.16888400	-0.15869400
H	-0.97480400	-1.50159400	1.92887600

H	1.39909400	-1.78736900	1.66169200
H	1.02443100	-1.11970100	-2.53434600
H	-1.38171100	-0.85109200	-2.29551500
N	-2.74839900	-1.02703500	-0.00819700
C	-3.32679500	-1.08356200	1.30361800
H	-2.91379100	-0.31472700	1.95961000
H	-4.39425500	-0.91549400	1.22878100
H	-3.16758800	-2.05688600	1.77070000
C	-3.56364600	-0.71664200	-1.15005700
H	-4.59286400	-0.60813600	-0.83014700
H	-3.25962600	0.21934700	-1.61955100
H	-3.52195800	-1.51135500	-1.89659100
C	3.53973000	-1.92690000	0.35617800
H	4.54061100	-1.98618100	-0.05286600
H	3.50988100	-1.14410900	1.11206000
H	3.27172700	-2.88305000	0.80675700
O	2.69506800	-1.62702800	-0.72224700

TCE:BZ2NH

E(RmPW+HF-B95) = -790.099637425 AU

C	0.59788500	-1.38179200	-0.32943500
C	-0.59786700	-1.38188100	0.32914500
C	-1.83676800	-1.39117500	-0.36112200
N	-2.86660200	-1.37527200	-0.87847000
C	-0.64859800	-1.44364400	1.74909800
N	-0.69725000	-1.51751800	2.89684400
C	0.64862300	-1.44323700	-1.74940000
N	0.69729300	-1.51682600	-2.89716400
C	1.83677400	-1.39121500	0.36085200
N	2.86659400	-1.37539200	0.87823200
C	-0.68244100	1.57750000	-1.20309300
C	0.69152100	1.57076500	-1.19030300
C	1.41212700	1.57794200	0.01268800
C	0.68242200	1.57716600	1.20340900
C	-0.69154000	1.57042900	1.19062100
C	-1.41214600	1.57794500	-0.01237000
H	-1.20601800	1.57439700	-2.14739600
H	1.20600100	1.57380800	2.14771100
N	2.78106900	1.63621600	0.02579000
N	-2.78107600	1.63622600	-0.02544600
H	-3.22846600	1.21591400	-0.82182300
H	-3.23896300	1.38857800	0.83279000
H	3.23891000	1.38890600	-0.83257200
H	3.22841700	1.21539700	0.82192900
H	1.22781000	1.55935800	-2.12825500
H	-1.22783000	1.55877200	2.12857000

TCE:BZ4O

E(RmPW+HF-B95) = -1137.31332110 AU

C	0.68238000	-0.00025800	1.86178100
C	-0.68247600	-0.00024000	1.86173500

C	-1.41731700	-1.21482800	1.91853100
N	-2.01734200	-2.19485500	1.98682400
C	-1.41733300	1.21432200	1.91893700
N	-2.01740400	2.19429100	1.98768500
C	1.41723000	-1.21483900	1.91870700
N	2.01728800	-2.19483100	1.98723800
C	1.41723300	1.21430400	1.91894000
N	2.01727400	2.19430200	1.98751100
C	1.20661900	0.70347000	-1.09541400
C	0.00004200	1.38558000	-1.09726300
C	-1.20654200	0.70348600	-1.09545200
C	-1.20656800	-0.70316900	-1.09568400
C	0.00000900	-1.38528000	-1.09764000
C	1.20659500	-0.70318600	-1.09556900
H	0.00005600	2.46117900	-1.10195100
H	-0.00000600	-2.46087800	-1.10262100
O	2.40741300	-1.28790600	-1.11439000
O	-2.40735900	1.28821500	-1.11416500
C	2.46090200	-2.67994400	-1.28284400
H	3.51308500	-2.93358200	-1.31905500
H	1.99920300	-3.20051300	-0.44681700
H	1.98197300	-2.97595600	-2.21663300
C	-2.46084100	2.68028500	-1.28235000
H	-3.51302100	2.93393400	-1.31854900
H	-1.99916600	3.20070200	-0.44621300
H	-1.98187500	2.97647500	-2.21606500
O	-2.40738400	-1.28784900	-1.11470600
O	2.40743600	1.28815600	-1.11419600
C	-2.46093000	-2.67988700	-1.28309000
H	-1.99902000	-3.20048100	-0.44720000
H	-3.51312400	-2.93351100	-1.31902000
H	-1.98223200	-2.97592400	-2.21699700
C	2.46099600	2.68023200	-1.28225300
H	1.99898200	3.20064700	-0.44630900
H	3.51319200	2.93387000	-1.31800100
H	1.98240500	2.97647500	-2.21615100

TCE:BZ2N

E(RmPW+HF-B95) = -947.231740271 AU

C	-0.49420100	1.71374400	0.47352500
C	0.49420400	1.71379200	-0.47362900
C	0.16782400	1.75007600	-1.85593500
N	-0.10677500	1.79129900	-2.97348200
C	1.86767300	1.74413600	-0.12832400
N	2.99364800	1.76363600	0.11937400
C	-1.86767700	1.74398100	0.12823000
N	-2.99365600	1.76355300	-0.11944500
C	-0.16783100	1.75021200	1.85582900
N	0.10672600	1.79155000	2.97338300
C	-0.68094100	-1.25492200	1.19315700
C	0.69298100	-1.27435700	1.19629400
C	1.42764800	-1.26924800	0.00268900
C	0.68094300	-1.25490900	-1.19308500

C	-0.69297700	-1.27442400	-1.19622200
C	-1.42764400	-1.26930900	-0.00261700
H	-1.18858700	-1.24675100	2.14380700
H	1.19859600	-1.26799800	2.14708300
H	1.18858800	-1.24671500	-2.14373500
H	-1.19859100	-1.26811100	-2.14701100
N	2.78592700	-1.27382300	-0.00287600
N	-2.78592300	-1.27391500	0.00294500
C	-3.49430200	-1.19364000	1.24861400
H	-3.22138100	-0.29677100	1.80731100
H	-4.55792000	-1.14694000	1.04933800
H	-3.30290500	-2.06461200	1.87777000
C	-3.49985200	-1.25083400	-1.24391500
H	-4.56348700	-1.21733900	-1.04186600
H	-3.24444500	-0.37228000	-1.83663200
H	-3.29270000	-2.14404200	-1.83572700
C	3.49432100	-1.19378600	-1.24855100
H	3.22150600	-0.29696300	-1.80737100
H	4.55794200	-1.14717300	-1.04927400
H	3.30284400	-2.06481800	-1.87760000
C	3.49986800	-1.25082500	1.24397800
H	4.56350800	-1.21756300	1.04191300
H	3.24465500	-0.37217900	1.83663800
H	3.29253300	-2.14395900	1.83583800

MPWB1K/6-31G(d) Cartesian coordinates and electronic energies of the five MCs between **ACE** and cyclic anhydride derivatives.

ACE:MA

E(RmPW+HF-B95) = -840.999839911 AU

C	2.84097100	-1.96371000	-0.65177600
C	3.11630700	-0.66090200	-0.97880800
C	2.36163000	0.38575800	-0.39988500
C	1.38336900	0.00117400	0.49914300
C	1.07708200	-1.32703000	0.83443500
C	1.81349000	-2.32166700	0.25154600
H	3.20793200	2.15064200	-1.33229800
H	3.42427100	-2.75163500	-1.10380500
H	3.90513900	-0.43549900	-1.68151800
C	2.46301800	1.77525000	-0.64586300
C	0.50202900	0.87773600	1.15222400
H	1.62896600	-3.36548000	0.45925400
C	0.61002200	2.21561600	0.88628100
C	1.60874600	2.64569000	-0.01814400
H	-0.05584500	2.94134500	1.32839300
H	1.69351900	3.70213800	-0.22286600
C	-0.05816900	-1.25921800	1.75260100
C	-0.39391100	0.03503200	1.94080700
H	-0.54707100	-2.10946400	2.19766500
H	-1.19637600	0.39641200	2.56193100
C	-1.42568700	-0.82057900	-1.38348200
C	-1.29522600	0.49557700	-1.39832700
C	-2.55149700	-1.15367200	-0.48822900
C	-2.33489000	1.06107400	-0.51342200
O	-2.99472900	-2.21150500	-0.18895200
O	-2.55892600	2.19191900	-0.23412800
O	-3.06562600	0.02167200	-0.01039500
H	-0.57069900	1.11378400	-1.89872300
H	-0.83929700	-1.57570900	-1.87482700

ACE:DCPA

E(RmPW+HF-B95) = -1913.88443163 AU

C	2.17504800	2.89392700	-0.44274400
C	0.87152900	3.26525400	-0.65678200
C	-0.16558000	2.65855100	0.08772400
C	0.22954300	1.70248400	1.00596800
C	1.55713400	1.31058200	1.23936700
C	2.54275100	1.91476300	0.50808000
H	-1.94152400	3.62693000	-0.69328000
H	2.95607100	3.37025700	-1.01626700
H	0.63978300	4.02387600	-1.39041900
C	-1.55792800	2.89232900	-0.00021400
C	-0.64086400	0.97157800	1.83121700
H	3.58456200	1.66000200	0.63308100
C	-1.98384400	1.20923200	1.72036300
C	-2.42181200	2.18622600	0.79654000

H	-2.71154000	0.66838300	2.30719300
H	-3.48180600	2.37033100	0.71124200
C	1.49609000	0.27145800	2.26453600
C	0.20576500	0.07310000	2.61242600
H	2.34590700	-0.25522900	2.66501800
H	-0.14997100	-0.63540500	3.34193800
C	0.51323700	-1.56773900	-0.45326600
C	-0.85231100	-1.37617700	-0.52327100
C	-1.41386600	-0.54674400	-1.46979800
C	-0.55345900	0.11897300	-2.32994600
C	0.81603300	-0.06265800	-2.25255900
C	1.37060400	-0.92604200	-1.31975800
C	0.77008800	-2.51285800	0.64836800
C	-1.45979000	-2.15487300	0.57092200
O	1.78257600	-2.98339500	1.04160600
O	-2.58884900	-2.24231000	0.91853500
O	-0.44476200	-2.81763000	1.20683000
Cl	3.06343600	-1.16168600	-1.26206600
Cl	-3.10612100	-0.34809800	-1.61551000
H	1.46597300	0.46972600	-2.92770300
H	-0.96373200	0.78595300	-3.07083200

ACE:TCPA

E(RmPW+HF-B95) = -2833.17081217 AU

C	2.36821000	-0.47180500	2.42154300
C	1.86742000	0.80524400	2.40016200
C	0.47719700	1.01357100	2.24856900
C	-0.29592400	-0.12707200	2.12481600
C	0.19945500	-1.44037200	2.13953100
C	1.54820400	-1.61554800	2.29055700
H	0.31738700	3.17553700	2.27320100
H	3.43207800	-0.61433900	2.53503700
H	2.53458000	1.64872100	2.50045400
C	-0.22066700	2.24258100	2.19037600
C	-1.69047600	-0.13983800	1.95660700
H	1.99867800	-2.59678500	2.30746600
C	-2.34230600	1.06242500	1.90092300
C	-1.58216500	2.24819400	2.02523600
H	-3.41015200	1.12947900	1.75510100
H	-2.09896300	3.19424000	1.97445500
C	-0.95950400	-2.30980100	1.95406100
C	-2.06995000	-1.54656400	1.85240400
H	-0.92677600	-3.38502500	1.90242200
H	-3.07464100	-1.90880900	1.71149300
C	-0.54262600	-1.06188000	-1.24160800
C	-1.12047600	0.18624600	-1.28284600
C	-0.36879100	1.33922600	-1.25751000
C	1.01454700	1.19387300	-1.14831300
C	1.60518600	-0.07480400	-1.11494900
C	0.82195200	-1.22815700	-1.17181000
C	-1.62990800	-2.05728100	-1.30888900
C	-2.58320700	-0.00774000	-1.32014300
O	-1.59400900	-3.23863300	-1.35274300

O	-3.46442200	0.78270000	-1.32628700
O	-2.80768100	-1.35650400	-1.33889900
Cl	1.51801700	-2.77978400	-1.14781900
Cl	3.30145300	-0.21595200	-1.03846000
Cl	1.99445100	2.58423000	-1.04859400
Cl	-1.09747100	2.86994700	-1.39856800

ACE:4NOPA

E(RmPW+HF-B95) = -737.130965244 AU

C	-1.95594900	2.51845800	-1.19902600
C	-2.53020300	1.72546300	-0.23717000
C	-1.73732100	1.21338100	0.81626300
C	-0.39606300	1.55346500	0.78680500
C	0.20921800	2.35635000	-0.19308000
C	-0.58165800	2.84974500	-1.19496100
H	-3.16723400	0.05263100	1.96269800
H	-2.57573700	2.90746700	-1.99280800
H	-3.58301700	1.49017900	-0.28732500
C	-2.13782400	0.36910800	1.87884200
C	0.56225100	1.12899000	1.72086600
H	-0.18463000	3.47752700	-1.97940000
C	0.15133700	0.31067500	2.73796300
C	-1.21271200	-0.05776200	2.79847500
H	0.83927600	-0.07033800	3.47788100
H	-1.53438100	-0.70490600	3.60029600
C	1.62643000	2.41790100	0.15575100
C	1.83397200	1.69641800	1.27917200
H	2.38009000	2.95014700	-0.40003000
H	2.78031600	1.55623800	1.77466800
C	1.41452800	-0.71143900	-1.28554300
C	1.07625700	-1.42707900	-0.16042900
C	-0.21181800	-1.84428800	0.08153600
C	-1.13415400	-1.47956800	-0.87766000
C	-0.81825400	-0.76693300	-2.02503800
C	0.48839200	-0.37517100	-2.24883600
C	2.85352500	-0.40231500	-1.19307300
C	2.28823700	-1.55322200	0.66594600
O	3.55722700	0.18618200	-1.94236700
O	2.44288500	-2.05557100	1.72790900
O	3.30936300	-0.94391300	-0.01843700
H	0.76776300	0.18828300	-3.12392200
H	-0.50450800	-2.38262700	0.96626400
H	-1.60982000	-0.51694500	-2.71033300
N	-2.53310100	-1.81085400	-0.64231900
O	-2.78706100	-2.49137400	0.32131300
O	-3.34810800	-1.37091700	-1.41748900

ACE:35DNPA

E(RmPW+HF-B95) = -941.526563646 AU

C	3.15932400	-0.48914700	1.31371800
C	2.62234600	0.75695100	1.52138900

C	1.24224800	0.89093600	1.80447200
C	0.51549400	-0.28624700	1.84530300
C	1.04826300	-1.56960100	1.63926800
C	2.38562700	-1.67185400	1.36435700
H	0.99950800	3.03876200	1.98108000
H	4.21166800	-0.57437100	1.08923900
H	3.25297400	1.63181800	1.46307600
C	0.50516100	2.07923400	2.01319300
C	-0.86493100	-0.37066100	2.08571500
H	2.86321900	-2.62422200	1.18707400
C	-1.55831200	0.79487600	2.28031500
C	-0.84708500	2.01519300	2.24353400
H	-2.62540600	0.80507200	2.44491200
H	-1.39546400	2.93383000	2.38617700
C	-0.07538500	-2.49520500	1.75494800
C	-1.19912500	-1.79096900	2.01760400
H	-0.01283700	-3.56467700	1.64376500
H	-2.18457400	-2.20296500	2.15880200
C	-0.56804700	-1.14910100	-1.31033200
C	-1.33516200	-0.03355000	-1.05431400
C	-0.72600600	1.21063400	-1.08813500
C	0.62741700	1.30329000	-1.32414900
C	1.35464600	0.14899200	-1.54682800
C	0.78490300	-1.10363600	-1.56527400
C	-1.43762800	-2.33399600	-1.24213600
C	-2.69258400	-0.53779500	-0.68187800
O	-1.18363800	-3.47135500	-1.45147300
O	-3.63609600	0.00565200	-0.22839200
O	-2.68044800	-1.89411200	-0.89442300
H	1.11093100	2.26515100	-1.33186600
H	1.37026600	-1.98739200	-1.75496000
N	-1.46410500	2.45608100	-0.94484600
O	-2.65449900	2.40193100	-1.10066500
O	-0.82085200	3.45176300	-0.71368600
N	2.78860300	0.27082400	-1.76995800
O	3.26164300	1.37919900	-1.73624000
O	3.40029600	-0.75050300	-1.96115600