On the effects of the basis set superposition error on the change of QTAIM charges in adduct formation. Application to complexes between morphine and cocaine and their main metabolites.

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SUPPORTING INFORMATION

Supplementary Table 1 B3LYP/6-31++G** 6d total energies, E, virial ratios, γ, and zero-point energy corrections, ZPE, for all the systems studied herein. Recovering errors from QTAIM atomic fragments for energies, E-$\Sigma E(\Omega)$, and electron populations, N-$\Sigma N(\Omega)$, are, respectively in kJ mol^{-1} and in au multiplied by 10^3. All the remaining values are in a.u. except ZPE which are in kJ mol^{-1}. The letters on each acronym correspond to: **M**, morphine; **H**, heroin; **C**, cocaine; and **E**, ecgonine methyl ester.

		E				$E - \Sigma E(\Omega)$				$N - \Sigma N(\Omega)$				$\gamma = -V / T$				ZPE	
Complex	Monomers	$E^X_X(X)$	$E^X_X(M)$	$E^X_M(M)$	$E^M_M(M)$	X^X_X	M^X_X	M^M_X	M^M_M	X^X_X	M^X_X	M^M_X	M^M_M	X^X_X	M^X_X	M^M_X	M^M_M	X^X_X	M^M_M
HE1	**E**	-1917.482893	-672.161951	-672.161463	-672.161793	-0.15	-0.41	-0.56	-0.28	0.1	-0.3	-0.6	-0.1	2.00931	2.00939	2.00940	2.00936	1868.37	747.66
	H		-1245.348544	-1245.348144	-1245.349645		0.09	1.45	1.13		0.3	-1.0	2.5		2.00931	2.00931	2.00929		1116.21
HE2	**E**	-1917.480451	-672.161872	-672.161414	-672.161793	0.27	-0.28	-0.60	-0.28	1.5	-0.1	-0.6	-0.1	2.00931	2.00939	2.00940	2.00936	1867.26	747.65
	H		-1245.345237	-1245.344774	-1245.349645		0.45	-0.10	0.81		1.7	0.8	1.7		2.00931	2.00932	2.00929		1116.22
MC1	**C**	-1956.567271	-1016.583026	-1016.582277	-1016.583159	0.05	0.05	-1.03	0.24	0.4	-1.1	-1.0	0.8	2.00935	2.00941	2.00943	2.00940	1911.83	987.62
	M		-940.015661	-940.014773	-940.014943		-0.58	-0.16	-0.44		0.2	-0.4	-0.6		2.00935	2.00937	2.00933		920.79
MC2	**C**	-1956.561552	-1016.581306	-1016.580618	-1016.583159	-0.20	-0.25	0.44	0.27	0.3	0.0	1.3	0.8	2.00935	2.00940	2.00942	2.00940	1910.40	987.61
	M		-940.012101	-940.011050	-940.011992		-0.04	0.93	-0.19		0.4	1.7	-0.2		2.00938	2.00939	2.00933		919.46
MC3	**C**	-1956.560776	-1016.583420	-1016.582932	-1016.583159	3.34	-1.57	0.11	0.38	-0.7	-2.3	0.4	1.0	2.00935	2.00941	2.00943	2.00940	1908.86	987.61
	M		-940.017558	-940.016789	-940.016991		-0.21	-0.12	-0.27		0.0	-0.2	-0.7		2.00934	2.00935	2.00933		920.79
MC4	**C**	-1956.560209	-1016.582686	-1016.582213	-1016.583159	0.01	-0.05	-0.19	0.29	0.8	0.5	0.0	0.9	2.00935	2.00940	2.00942	2.00940	1909.42	987.62
	M		-940.017266	-940.016541	-940.016991		0.09	0.11	-0.50		0.7	-0.0	-0.8		2.00936	2.00938	2.00933		920.79
ME1	**E**	-1612.140055	-672.162726	-672.162257	-672.162493	-0.58	0.16	-0.32	-0.34	-0.3	0.4	-0.2	-0.4	2.00934	2.00938	2.00939	2.00936	1671.51	748.04
	M		-940.012077	-940.011528	-940.012402		-0.29	0.95	-0.02		-0.1	1.9	0.5		2.00937	2.00937	2.00933		920.38
ME2	**E**	-1612.143016	-672.161694	-672.161267	-672.161793	0.24	0.05	-0.59	-0.25	0.7	0.4	-0.7	-0.1	2.00934	2.00939	2.00940	2.00936	1671.69	747.67
	M		-940.017055	-940.016492	-940.016991		0.06	-0.56	-0.37		0.4	-0.5	-0.8		2.00937	2.00937	2.00933		920.78
ME3	**E**	-1612.139209	-672.162126	-672.161502	-672.162493	-0.31	-0.98	-0.27	-0.35	0.1	-1.0	-0.1	-0.4	2.00933	2.00936	2.00939	2.00936	1671.21	748.03
	M		-940.011963	-940.011206	-940.012402		-0.60	0.20	-0.02		-0.2	0.5	0.5		2.00937	2.00938	2.00933		920.38
ME4	**E**	-1612.139783	-672.162671	-672.162063	-672.162493	-0.48	0.22	-0.93	-0.34	-0.7	0.5	-1.2	-0.4	2.00934	2.00938	2.00939	2.00936	1671.71	748.02
	M		-940.015068	-940.014529	-940.014943		-0.48	0.29	-0.44		-0.3	0.7	-0.6		2.00936	2.00937	2.00933		920.79
ME5	**E**	-1612.138217	-672.162147	-672.161600	-672.162493	0.04	-0.88	-0.66	-0.33	1.1	-1.0	-0.7	-0.4	2.00933	2.00936	2.00939	2.00936	1671.61	748.04
	M		-940.015240	-940.014611	-940.014943		1.17	-0.51	-0.38		2.5	-0.4	-0.5		2.00936	2.00937	2.00933		920.79

Supplementary Table 2 The atomic property variations, $P(\Omega)$, shown are defined as follows: $\Delta_{def}P(\Omega)=(P_X^M(\Omega_M)-P_M^M(\Omega_M))$,$-\Delta_{BSSE}P(\Omega)=(P_X^X(\Omega_M)-P_X^M(\Omega_M))$, and $\Delta_b^{CP}P(\Omega)=(P_X^X(\Omega_X)-P_X^X(\Omega_M))$. These properties are the atomic electron population, $N(\Omega)$, the atomic energy, $E(\Omega)$, and the atomic volume, $v(\Omega)$. All the values are in au but energy variations are in kJ mol^{-1}. To nomenclature purposes see Figure 1 in manuscript. Moreover, the acronyms T, C, G$^-$, G$^+$, A$^-$, and A$^+$ respectively correspond to antiperiplanar orientation, synperiplanar, - synclinal, + synclinal, - anticlinal, and + anticlinal.

Supplementary Table 2.1a Integrated properties of ecgonine methyl ester in HE1.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.7246	-37.91387	46.95	-4.4	0.2	7.1	0	0	0	-110	23	8
H1	0.9635	-0.62342	45.73	-0.5	0.0	0.9	0	0	-1	-31	-21	-72
C2	5.9373	-38.07088	48.07	-2.7	0.1	5.5	0	0	0	-42	-35	-49
H2	0.9537	-0.61744	44.53	-3.0	0.0	-3.8	2	0	3	16	-5	179
C1'	4.3834	-37.02715	33.75	-10.4	-0.2	5.6	3	0	1	141	-32	-43
O1'	9.2095	-75.99866	123.29	-9.6	1.5	16.1	1	0	0	219	-40	2
O2'	9.0940	-75.97442	100.21	11.1	0.9	9.6	-2	0	3	483	-64	189
C3'	5.5379	-37.75967	62.58	-2.0	-0.5	9.6	-1	0	-1	-87	-137	-33
Ht(C3')	0.9458	-0.61142	45.56	-0.5	0.0	-2.7	1	0	3	45	-56	148
Hg+(C3')	0.9485	-0.61085	45.59	-2.4	0.1	6.1	2	0	-5	153	29	-388
Hg-(C3')	0.9487	-0.61070	45.77	0.7	0.0	-7.2	-1	0	7	-91	5	481
C3	5.4188	-37.68551	41.34	23.5	-2.1	18.0	-9	0	-6	24	39	-126
H3	1.0075	-0.64898	45.72	-1.0	0.1	-2.9	1	0	3	313	11	285
O3	9.1651	-75.84731	121.25	18.3	-1.4	-74.0	4	0	45	402	-119	208
H(O3)	0.3672	-0.33302	14.05	8.2	-0.4	46.3	0	1	-30	198	100	-6294
C4	5.9403	-38.05421	55.44	0.2	-0.6	9.1	-1	0	-1	27	-8	-51
H4a	0.9733	-0.62014	45.20	1.3	0.0	-3.5	-1	0	3	167	-16	274
H4e	0.9886	-0.62439	48.65	-0.2	0.1	-1.8	-1	0	2	-199	45	184
C5	5.7212	-37.90904	48.01	-4.5	0.0	7.0	0	0	0	32	-96	10
H5	0.9663	-0.62392	46.00	0.0	0.0	-0.9	0	0	1	17	10	76
C6	5.9357	-38.01419	58.09	-5.0	0.1	8.6	0	0	0	44	27	-12
H6a	0.9855	-0.62525	47.27	-0.6	0.1	-3.8	0	0	4	35	6	278
H6e	0.9900	-0.62917	47.53	0.2	0.0	1.0	0	0	-1	3	19	-46
C7	5.9352	-38.01323	58.07	-5.2	0.0	8.8	0	0	0	-22	29	-4
H7e	0.9851	-0.62725	47.34	-0.5	-0.1	2.2	0	0	-2	-101	59	-131
H7a	0.9829	-0.62436	46.65	-0.4	0.0	-2.3	0	0	2	120	-23	167
N8	8.0348	-55.35619	59.66	-1.1	1.0	12.7	-2	0	0	13	10	-17
H8	0.4828	-0.39983	16.93	-3.6	0.1	-1.5	3	0	1	397	10	26
C8	5.6624	-37.85359	64.00	-5.5	-0.6	7.1	2	0	0	61	-75	23
Ha-(C8)	0.9443	-0.60651	45.83	0.5	0.0	1.0	0	0	-1	-41	16	-31
Ha+(C8)	0.9434	-0.60601	45.84	-0.1	0.0	2.1	0	0	-2	-16	12	-108
Hc(C8)	0.9558	-0.61444	44.34	0.5	0.0	1.1	-1	0	-1	-48	-11	-48

Supplementary Table 2.1b Integrated properties of heroin in HE1.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b{}^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b{}^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b{}^{CP}v(\Omega)\cdot10^3$
C1	5.9924	-38.03219	84.16	-5.9	0.1	2.4	0	0	-4	-17	-28	-231
H1	0.9721	-0.61544	48.56	-0.1	0.0	8.2	0	0	-8	-5	9	-559
C2	5.9643	-38.03338	80.24	-4.3	0.3	1.7	0	0	-3	-4	-63	-134
H2	0.9380	-0.60767	43.55	0.1	0.0	7.3	0	0	-7	-71	31	-467
C3	5.5077	-37.77227	61.89	0.2	0.1	2.8	0	0	-2	264	-42	-67
O3	9.1183	-76.00082	99.45	-13.7	0.7	2.2	1	0	-2	-180	47	-76
C1'	4.4426	-37.04457	38.40	-1.7	0.1	-1.6	0	0	1	25	13	14
O1'	9.2210	-76.00425	126.68	-0.8	0.9	-3.8	-1	0	4	-551	-27	168
C2'	5.9234	-38.01355	70.15	-2.2	0.3	-0.1	0	0	0	81	8	8
Ha-(C2')	0.9517	-0.60264	46.64	4.5	0.0	7.5	-1	0	-7	186	-13	-440
Ha+(C2')	0.9503	-0.60161	46.68	-5.0	0.0	-0.3	1	0	0	-285	-54	-5
Hc(C2')	0.9500	-0.60797	44.75	1.1	0.0	-2.9	-1	0	3	56	6	109
C4	5.4916	-37.84845	58.03	-6.9	-0.1	-7.1	7	0	6	150	16	147
O	8.9971	-75.78898	103.84	1.9	0.2	-6.1	-3	0	5	-935	-22	360
C5	5.5587	-37.88132	41.44	13.7	2.1	0.6	-12	-1	0	-372	-105	16
H5	0.9754	-0.64581	41.37	-1.3	0.0	4.4	-1	0	-4	-273	50	-194
C6	5.4845	-37.74557	44.38	-17.2	-0.7	-17.0	21	-1	10	1652	-86	90
H6	0.9379	-0.61313	42.63	15.1	0.1	-14.7	-8	0	10	443	-3	342
O6	9.0779	-75.93062	100.53	-110.0	-1.5	25.3	18	0	-10	-799	-26	-770
C1”	4.4546	-37.06264	38.81	28.7	-1.9	11.7	-12	0	-2	-21	-7	-225
O1”	9.2008	-76.01367	133.66	126.2	4.9	-80.7	-10	0	34	1475	-145	-6645
C2”	5.9207	-38.00503	70.64	-4.0	-5.8	-13.0	0	0	7	16	-25	259
Hc(C2”)	0.9550	-0.60709	46.54	2.8	-0.4	-1.5	-1	1	-8	21	100	-2960
Ha-(C2”)	0.9657	-0.60952	47.29	1.4	-0.1	11.5	0	0	-10	124	-23	-676
Ha+(C2”)	0.9560	-0.60297	47.27	-9.6	-0.1	14.7	5	0	-13	0	55	-942
C7	6.0076	-38.06548	79.77	3.1	-0.4	-0.9	-2	0	5	107	49	440
H7	0.9281	-0.59796	45.11	-1.9	0.0	-2.5	1	0	2	3	0	112
C8	6.0257	-38.04535	83.66	-6.8	-0.1	6.9	0	0	-8	-113	-38	-605
H8	0.9585	-0.60873	47.88	-0.9	0.0	9.1	0	0	-9	7	17	-610
C9	5.7588	-37.89155	48.46	-1.3	0.4	1.5	-1	0	0	-68	-14	34
H9	0.9683	-0.62637	46.15	0.3	0.0	5.1	0	0	-5	-4	-6	-352
C10	5.9300	-37.99894	58.42	-4.5	-0.3	-0.5	0	-1	0	-65	-159	47
H10e	0.9934	-0.62968	46.38	-0.1	0.0	7.2	0	0	-7	-25	40	-346
H10a	0.9585	-0.61233	46.67	0.4	0.0	3.2	0	0	-3	-69	20	-222
C11	6.0159	-38.10707	68.98	-3.9	0.0	2.7	1	0	-2	-31	-6	-62
C12	6.0435	-38.26481	59.84	0.7	-0.2	0.7	0	0	0	-70	-25	30
C13	5.9564	-38.12502	40.98	7.1	0.5	1.7	2	0	0	299	8	15
C14	5.9471	-38.05244	49.20	-2.2	0.2	-0.8	0	0	0	-3	-41	3
H14	1.0244	-0.66325	42.16	1.4	0.0	0.1	-1	0	0	-29	-42	44
C15	5.9247	-38.02332	55.81	2.0	0.6	-0.6	-1	1	1	81	53	-30
H15e	0.9557	-0.61244	44.92	-1.2	0.0	-2.0	1	0	2	172	-82	97
H15a	0.9975	-0.63012	48.16	0.9	0.0	-8.5	0	0	8	177	52	416
C16	5.7297	-37.90167	53.81	0.1	0.3	2.2	0	0	-1	27	56	-1
H16e	0.9587	-0.61828	45.79	0.0	0.0	2.5	0	0	-2	45	-26	-106
H16a	0.9531	-0.61972	42.44	-1.4	0.0	4.5	1	0	-4	16	-41	-172
N17	7.9558	-55.22503	58.84	2.2	0.3	-0.3	-1	0	1	53	-24	-35
H17	0.5658	-0.45138	27.23	1.0	0.0	-1.3	-1	0	1	25	1	9
C17	5.6728	-37.86294	62.93	-5.3	0.2	-1.7	3	0	1	4	-12	104
Ha+(C17)	0.9424	-0.60576	45.54	0.3	0.0	5.1	0	0	-5	-81	-30	-254
Ha-(C17)	0.9406	-0.60540	45.35	0.1	0.0	3.6	0	0	-3	-28	30	-172
Hc(C17)	0.9447	-0.60935	43.87	0.8	0.0	2.9	-1	0	-3	74	-41	-162

Supplementary Table 2.2a Integrated properties of ecgonine methyl ester in HE2.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.7246	-37.91387	46.95	-3.5	0.6	6.8	0	0	0	-78	67	4
H1	0.9635	-0.62342	45.73	-0.5	0.0	0.5	0	0	0	17	-1	-40
C2	5.9373	-38.07088	48.07	-2.2	0.0	5.0	1	0	0	49	-7	-31
H2	0.9537	-0.61744	44.53	-2.5	0.0	-4.7	2	0	4	80	-16	264
C1'	4.3834	-37.02715	33.75	-13.0	-0.3	6.9	5	0	1	184	-4	-42
O1'	9.2095	-75.99866	123.29	-13.3	1.2	16.4	0	0	0	-239	48	-21
O2'	9.0940	-75.97442	100.21	11.5	0.1	9.2	-2	0	4	463	-79	232
C3'	5.5379	-37.75967	62.58	-3.0	-0.3	8.9	0	0	-1	-35	-73	3
Ht(C3')	0.9458	-0.61142	45.56	-0.3	0.0	-3.7	1	0	3	1	37	167
Hg+(C3')	0.9485	-0.61085	45.59	-1.7	0.1	5.4	1	0	-5	33	4	-289
Hg-(C3')	0.9487	-0.61070	45.77	0.6	0.0	-4.8	-1	0	4	-107	-18	327
C3	5.4188	-37.68551	41.34	26.9	-0.8	20.5	-13	0	-8	-134	49	-166
H3	1.0075	-0.64898	45.72	-1.5	0.1	-3.4	2	0	4	159	17	312
O3	9.1651	-75.84731	121.25	16.7	-1.8	-81.0	7	0	48	630	-248	1119
H(O3)	0.3672	-0.33302	14.05	10.3	-0.6	47.8	0	1	-33	181	126	-7197
C4	5.9403	-38.05421	55.44	-1.6	-0.3	8.4	-2	0	-1	-119	65	-74
H4a	0.9733	-0.62014	45.20	0.4	0.0	-2.7	-1	0	3	-109	13	233
H4e	0.9886	-0.62439	48.65	1.0	0.1	-4.0	-1	0	4	-155	27	345
C5	5.7212	-37.90904	48.01	-3.1	-0.2	6.7	0	0	0	5	-9	-7
H5	0.9663	-0.62392	46.00	0.3	0.0	-1.6	0	0	2	56	-17	76
C6	5.9357	-38.01419	58.09	-3.8	-0.1	8.5	0	0	0	121	-94	-13
H6a	0.9855	-0.62525	47.27	-0.2	0.1	-4.5	0	0	4	73	83	311
H6e	0.9900	-0.62917	47.53	0.1	0.0	0.0	0	0	0	-14	-23	-8
C7	5.9352	-38.01323	58.07	-4.2	0.0	8.7	0	0	0	24	-66	-23
H7e	0.9851	-0.62725	47.34	-0.1	0.0	1.3	0	0	-1	-31	-27	-57
H7a	0.9829	-0.62436	46.65	-1.4	0.1	-2.6	1	0	3	45	23	188
N8	8.0348	-55.35619	59.66	-4.9	0.8	12.3	0	0	0	-18	-13	1
H8	0.4828	-0.39983	16.93	-1.6	0.0	-0.6	1	0	0	106	-6	7
C8	5.6624	-37.85359	64.00	-4.3	-0.4	7.0	1	0	0	71	-50	13
Ha-(C8)	0.9443	-0.60651	45.83	0.2	0.0	0.8	0	0	-1	-29	52	-50
Ha+(C8)	0.9434	-0.60601	45.84	-0.4	0.0	2.1	0	0	-2	21	-40	-104
Hc(C8)	0.9558	-0.61444	44.34	0.4	0.0	0.5	0	0	0	-5	28	-73

Supplementary Table 2.2b Integrated properties of heroin in HE2.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.9924	-38.03219	84.16	-1.9	0.0	2.7	-2	0	-2	-148	-3	-129
H1	0.9721	-0.61544	48.56	0.2	0.0	2.8	-1	0	-3	-78	-49	-228
C2	5.9643	-38.03338	80.24	13.3	-0.6	1.3	-11	0	4	-1619	-58	128
H2	0.9380	-0.60767	43.55	13.3	0.1	-18.0	-24	0	15	-3676	5	798
C3	5.5077	-37.77227	61.89	1.0	-0.6	-31.8	25	0	20	2578	-75	614
O3	9.1183	-76.00082	99.45	-136.8	-1.0	31.5	25	0	-10	-1874	13	-443
C1'	4.4426	-37.04457	38.40	44.7	-3.4	12.0	-19	0	-1	-190	-52	-301
O1'	9.2210	-76.00425	126.68	132.1	2.8	-94.6	-13	0	36	958	-264	-7451
C2'	5.9234	-38.01355	70.15	-10.2	-6.2	-9.6	0	-1	6	-403	-177	262
Ha-(C2')	0.9517	-0.60264	46.64	-5.5	-0.1	15.9	5	0	-15	389	-62	-942
Ha+(C2')	0.9503	-0.60161	46.68	-4.2	-0.1	14.6	3	0	-13	87	85	-909
Hc(C2')	0.9500	-0.60797	44.75	1.7	-0.3	-1.4	-1	1	-6	-56	137	-1896
C4	5.4916	-37.84845	58.03	6.1	-0.2	10.4	1	0	-7	2349	15	-267
O	8.9971	-75.78898	103.84	-8.0	0.8	0.3	-2	0	0	737	-53	3
C5	5.5587	-37.88132	41.44	-6.9	0.3	-6.5	5	0	4	29	50	80
H5	0.9754	-0.64581	41.37	-2.1	0.0	1.3	0	0	-1	-305	-41	-55
C6	5.4845	-37.74557	44.38	11.9	0.5	4.1	-8	0	-2	-799	-65	18
H6	0.9379	-0.61313	42.63	-12.5	0.0	3.5	12	0	-3	1395	6	-198
O6	9.0779	-75.93062	100.53	-10.9	1.1	1.0	-1	0	-2	-236	62	-144
C1”	4.4546	-37.06264	38.81	-7.5	0.6	-3.7	2	1	2	53	206	28
O1”	9.2008	-76.01367	133.66	-3.2	1.1	-0.5	0	0	1	370	28	58
C2”	5.9207	-38.00503	70.64	-1.8	0.5	0.5	0	0	0	46	29	22
Hc(C2”)	0.9550	-0.60709	46.54	1.2	0.0	0.8	0	0	-1	117	-34	-72
Ha-(C2”)	0.9657	-0.60952	47.29	-5.7	0.0	-0.9	1	0	1	-331	-28	49
Ha+(C2”)	0.9560	-0.60297	47.27	5.8	0.0	6.7	-3	0	-6	14	43	-426
C7	6.0076	-38.06548	79.77	-3.2	0.2	1.1	-1	0	-2	-61	-7	-134
H7	0.9281	-0.59796	45.11	2.3	0.0	7.4	-2	0	-7	-96	10	-424
C8	6.0257	-38.04535	83.66	-2.3	0.2	-0.6	-1	0	0	-287	66	9
H8	0.9585	-0.60873	47.88	0.5	0.0	6.4	-1	0	-6	-17	-13	-444
C9	5.7588	-37.89155	48.46	1.5	0.6	0.3	0	0	0	25	-28	48
H9	0.9683	-0.62637	46.15	0.2	0.0	8.0	-1	0	-7	-67	-35	-469
C10	5.9300	-37.99894	58.42	-0.2	0.1	-1.2	1	0	1	94	-74	57
H10e	0.9934	-0.62968	46.38	0.4	0.1	4.2	-1	0	-4	-37	0	-227
H10a	0.9585	-0.61233	46.67	-0.7	0.0	7.0	0	0	-6	-145	83	-452
C11	6.0159	-38.10707	68.98	-1.4	0.3	3.9	0	0	-4	138	49	-253
C12	6.0435	-38.26481	59.84	8.7	0.3	3.3	3	0	-4	603	-2	-106
C13	5.9564	-38.12502	40.98	14.2	0.1	0.8	0	0	-1	123	42	-8
C14	5.9471	-38.05244	49.20	-1.7	0.3	1.4	1	0	0	58	-29	35
H14	1.0244	-0.66325	42.16	-4.5	0.0	4.8	2	0	-4	-245	16	-238
C15	5.9247	-38.02332	55.81	5.1	0.1	0.8	-3	0	0	-52	-12	-17
H15e	0.9557	-0.61244	44.92	-11.6	0.0	-5.2	11	0	4	742	-4	243
H15a	0.9975	-0.63012	48.16	-0.7	0.0	7.5	0	0	-7	33	-65	-401
C16	5.7297	-37.90167	53.81	3.3	0.0	2.3	-2	0	-1	65	-63	-61
H16e	0.9587	-0.61828	45.79	0.1	0.0	4.4	0	0	-4	32	-25	-231
H16a	0.9531	-0.61972	42.44	-0.1	0.0	-8.2	1	0	7	272	17	341
N17	7.9558	-55.22503	58.84	-9.9	0.6	-1.5	1	0	2	0	-7	68
H17	0.5658	-0.45138	27.23	-0.2	0.0	6.4	0	0	-4	-42	-34	-237
C17	5.6728	-37.86294	62.93	-3.9	0.1	-0.7	2	0	1	278	-79	21
Ha+(C17)	0.9424	-0.60576	45.54	1.5	0.0	5.8	-1	0	-5	-44	-11	-282
Ha-(C17)	0.9406	-0.60540	45.35	0.4	0.0	4.0	0	0	-4	-25	-5	-227
Hc(C17)	0.9447	-0.60935	43.87	1.4	0.0	-5.2	-1	0	4	-51	66	220

Supplementary Table 2.3a Integrated properties of cocaine in MC1.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.7217	-37.91513	46.87	-3.1	2.2	4.8	-1	1	-2	-63	147	-150
H1	0.9599	-0.62192	45.51	-0.6	0.4	5.6	0	0	-5	-50	21	-313
C2	5.9346	-38.06797	48.10	-0.3	-0.7	7.3	0	0	0	89	-110	4
H2	0.9493	-0.61574	44.25	-0.6	0.4	-1.0	0	0	1	57	-39	53
C1'	4.3826	-37.02931	34.00	6.3	0.4	7.0	-3	0	-2	-20	-27	-21
O1'	9.2058	-76.00379	123.22	-15.1	7.1	12.2	1	1	-5	4	87	-394
O2'	9.0952	-75.97521	101.14	1.9	2.4	10.6	-1	0	2	-26	182	-144
C3'	5.5449	-37.76596	63.11	-7.8	2.9	-2.1	4	-1	4	221	-35	116
Ht(C3')	0.9390	-0.60856	45.15	1.0	0.7	2.6	-1	-1	-2	11	-91	-156
Hg+(C3')	0.9438	-0.60893	45.26	-0.2	-0.7	7.6	0	1	-7	-92	145	-591
Hg-(C3')	0.9495	-0.61104	46.74	1.1	-0.8	0.1	-1	0	0	321	-33	32
C3	5.5144	-37.76491	41.28	-1.8	-5.9	-4.7	11	0	9	648	48	102
H3	0.9511	-0.62938	38.82	8.0	-0.2	-11.0	-4	-1	7	556	-440	-321
O3	9.0940	-75.96156	94.52	-74.3	2.9	27.9	14	0	-8	-1038	427	-751
O1"	9.2315	-76.01030	125.81	109.3	-7.0	-79.8	-12	0	43	2204	-195	-5708
C1"	4.4857	-37.08595	39.92	11.3	-9.3	22.7	-9	0	1	-273	18	-145
C1r	5.9883	-38.09351	71.99	-5.1	1.0	13.1	-1	1	-2	-120	27	34
C2r	5.9847	-38.06890	80.66	-0.8	-3.2	5.3	-1	-1	3	9	40	-77
H2r	0.9600	-0.61440	45.67	0.5	0.7	-19.8	-1	0	19	9	-48	1225
C3r	5.9817	-38.05246	82.90	-3.9	-0.9	8.8	0	0	-2	194	-108	-169
H3r	0.9676	-0.61568	47.77	-0.4	0.1	0.9	0	0	-1	42	15	-98
C4r	5.9819	-38.05524	82.08	-3.1	1.4	7.4	1	0	-6	100	110	-580
H4r	0.9567	-0.61171	47.07	-1.1	0.1	12.0	1	0	-11	25	-15	-797
C5r	5.9817	-38.05256	82.86	-6.6	2.1	10.4	1	0	-7	73	-36	-454
H5r	0.9668	-0.61536	47.70	-2.5	0.5	13.4	2	0	-13	101	-40	-970
C6r	5.9853	-38.06673	80.56	-6.2	0.4	9.3	1	0	-6	2	8	-436
H6r	0.9676	-0.62101	47.12	-4.8	0.2	10.0	3	1	-10	318	78	-681
C4	5.9322	-38.05011	55.08	9.1	-1.7	7.1	-2	0	0	165	36	-175
H4a	0.9743	-0.62061	45.41	3.2	-0.8	2.3	-3	0	-2	-105	-104	35
H4e	0.9615	-0.61556	46.15	-2.7	-0.6	-7.7	4	1	4	1052	269	-89
C5	5.7204	-37.91147	48.01	-1.6	-1.0	11.3	-1	1	-3	-103	94	-26
H5	0.9623	-0.62236	45.76	-0.4	0.0	2.4	0	0	-2	12	68	-135
C6	5.9450	-38.02379	58.63	1.1	-2.7	-10.8	0	-1	9	171	-28	374
H6a	0.9433	-0.60925	42.63	1.1	0.7	22.8	0	0	-25	10	-3	-3408
H6e	0.9930	-0.63031	47.79	1.0	-0.4	-1.8	-1	0	2	-63	30	188
C7	5.9361	-38.01588	58.09	-2.3	1.6	5.0	0	0	0	91	-36	31
H7e	0.9847	-0.62729	47.27	0.0	0.3	2.3	0	0	-2	-33	-25	-175
H7a	0.9817	-0.62365	46.73	1.9	-0.4	-5.7	-1	0	6	143	-136	642
N8	8.0341	-55.35806	59.70	-4.8	6.5	3.3	0	-1	1	15	99	-96
H8	0.4851	-0.40157	17.12	0.7	-1.3	0.7	0	1	-1	38	101	-117
C8	5.6642	-37.85724	63.99	-5.0	0.2	4.2	2	-1	1	151	-91	38
Ha-(C8)	0.9421	-0.60559	45.58	0.6	0.0	3.1	-1	0	-3	17	-114	-213
Ha+(C8)	0.9419	-0.60538	45.76	0.0	0.2	4.9	0	0	-4	-5	1	-274
Hc(C8)	0.9535	-0.61355	44.20	0.5	0.1	1.3	-1	0	-1	25	-15	-82

Supplementary Table 2.3b Integrated properties of morphine in MC1.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.9923	-38.03414	83.83	-5.2	-0.2	0.4	0	0	-2	-89	33	-60
H1	0.9709	-0.61502	48.52	-0.4	0.0	5.6	0	0	-5	24	-72	-332
C2	5.9785	-38.03813	82.72	-4.4	-0.5	0.4	0	0	0	30	24	-26
H2	0.9397	-0.60275	46.08	0.2	0.1	3.3	0	0	-3	-9	40	-209
C3	5.4166	-37.72356	59.40	-8.3	-0.9	-2.9	2	0	3	61	39	110
O3	9.1316	-75.88167	121.93	-1.7	3.9	-1.3	-2	0	-1	27	-41	-32
H(O3)	0.3869	-0.34748	20.20	-0.8	0.3	-7.1	0	0	5	-40	32	247
C4	5.5705	-37.89597	60.48	-10.8	2.2	-4.8	5	-1	4	78	14	93
O	9.0173	-75.77209	106.07	13.8	1.2	-3.7	-4	1	7	57	28	390
C5	5.5650	-37.88149	41.75	0.2	-0.8	-0.4	-1	-1	2	-112	-80	60
H5	0.9855	-0.64938	42.67	-1.6	-0.7	8.1	0	0	-8	-66	-111	216
C6	5.4160	-37.68826	44.54	-4.9	-7.8	5.3	7	0	0	362	-45	-114
H6	0.9807	-0.63058	47.84	2.8	1.2	-14.5	-1	0	11	11	28	609
O6	9.1622	-75.82916	124.98	55.1	-0.1	-115.9	-6	-1	75	247	-328	3259
H(O6)	0.3745	-0.33917	14.27	3.6	-1.5	58.6	3	1	-45	389	283	-8905
C7	6.0290	-38.07800	81.18	-3.5	-7.5	5.8	-1	-1	-1	-128	113	125
H7	0.9534	-0.60740	47.08	-1.3	1.1	-11.4	0	0	10	33	-101	800
C8	6.0265	-38.04937	83.61	-7.1	-3.3	4.9	0	0	-5	-38	-88	-196
H8	0.9626	-0.61027	48.23	-0.8	0.1	3.0	1	0	-3	55	-56	-219
C9	5.7593	-37.89440	48.40	-1.9	0.7	2.0	-1	-1	0	1	1	58
H9	0.9722	-0.62802	46.42	-0.4	0.3	3.6	0	0	-3	-42	48	-259
C10	5.9262	-37.99913	58.23	-5.0	1.1	-0.4	0	0	0	7	-27	76
H10e	0.9934	-0.63002	46.33	-1.1	-0.2	6.5	0	0	-6	-107	73	-304
H10a	0.9673	-0.61604	47.35	-0.3	0.1	-0.3	0	0	0	-15	-12	37
C11	6.0215	-38.10776	69.53	-3.4	-0.4	1.0	0	0	-2	-35	20	-177
C12	6.0427	-38.26755	59.17	-2.4	3.0	-0.6	0	0	-1	-7	34	-7
C13	5.9577	-38.12462	41.10	0.6	3.2	-2.6	1	-1	0	90	47	-41
C14	5.9463	-38.05378	49.09	-3.6	-0.4	0.7	0	0	-1	-87	12	-48
H14	1.0267	-0.66311	42.68	1.2	-1.5	3.1	0	0	-2	141	-115	70
C15	5.9253	-38.02542	55.68	-1.7	2.1	-2.7	0	0	0	43	54	-128
H15e	0.9580	-0.61375	44.83	-0.4	0.3	-2.2	0	0	1	-6	51	6
H15a	1.0098	-0.63487	48.99	-0.1	0.1	-3.0	0	0	3	28	52	137
C16	5.7291	-37.90338	53.84	-1.8	1.3	1.0	-1	1	-1	-56	78	-37
H16e	0.9598	-0.61879	45.90	-0.6	0.1	4.5	0	0	-4	-2	-34	-209
H16a	0.9437	-0.61589	41.75	-0.2	0.2	1.6	0	0	-2	133	23	-164
N17	7.9538	-55.22399	58.76	1.4	-0.7	1.7	-1	1	0	-14	108	-141
H17	0.5694	-0.45352	27.52	0.3	0.1	0.6	0	0	-1	10	-6	-36
C17	5.6744	-37.86579	62.84	-5.7	2.0	-2.3	2	0	1	-48	202	-15
Ha+(C17)	0.9440	-0.60656	45.51	0.1	0.3	3.4	0	0	-3	-46	72	-301
Ha-(C17)	0.9406	-0.60545	45.45	0.0	0.1	4.7	0	0	-4	-8	36	-166
Hc(C17)	0.9382	-0.60672	43.51	0.3	-0.3	1.6	0	0	-2	22	-9	-76

Supplementary Table 2.4a Integrated properties of cocaine in MC2.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.7195	-37.91069	46.70	7.5	2.0	6.0	-3	0	-1	-257	57	-35
H1	0.9645	-0.62385	45.80	3.4	0.0	-3.1	-3	0	3	-228	10	164
C2	5.9319	-38.06967	47.77	-4.8	-1.8	8.4	-2	0	-1	-342	-42	36
H2	0.9488	-0.61727	43.63	-8.9	-0.2	3.9	4	0	-4	-296	10	-269
C1'	4.3828	-37.02820	33.95	11.7	-6.2	11.1	-7	0	2	-41	-25	-58
O1'	9.2373	-76.00443	123.87	49.9	1.2	-48.6	2	0	27	4811	-118	-4335
O2'	9.0936	-75.97954	100.40	-17.1	1.7	18.9	6	0	-7	-433	50	-354
C3'	5.5329	-37.75816	62.76	8.2	1.4	3.9	-6	0	0	10	-16	-47
Ht(C3')	0.9373	-0.60778	45.08	-4.7	0.1	11.1	4	0	-10	269	-43	-536
Hg+(C3')	0.9557	-0.61374	46.02	-0.2	0.0	-5.9	0	0	5	-46	4	280
Hg-(C3')	0.9578	-0.61403	47.49	-1.6	0.0	-6.0	3	0	5	654	62	343
C3	5.4946	-37.75608	40.62	8.7	0.0	2.1	-1	0	1	73	7	52
H3	0.9510	-0.62855	39.82	-5.5	-0.1	4.6	6	0	-4	936	11	-157
O3	9.0866	-75.93920	95.43	7.7	2.9	4.4	-4	0	4	-529	-46	124
O1"	9.2010	-76.01626	128.99	-7.4	3.2	11.1	1	0	-1	-406	-93	-20
C1"	4.4954	-37.09603	40.33	-4.9	0.4	2.9	0	1	1	-125	70	60
C1r	5.9911	-38.09554	72.13	-1.5	1.3	3.8	0	0	1	6	-7	78
C2r	5.9838	-38.06770	80.69	-1.7	1.8	4.4	0	0	0	107	-96	-8
H2r	0.9425	-0.60723	44.55	-0.7	0.1	0.9	1	0	-1	82	18	-36
C3r	5.9826	-38.05211	82.92	-2.2	1.8	5.3	0	0	-1	141	-140	-57
H3r	0.9646	-0.61450	47.53	-0.2	0.0	4.0	0	0	-4	16	-39	-256
C4r	5.9861	-38.05540	82.52	-2.0	1.8	5.4	0	0	-1	65	47	-46
H4r	0.9635	-0.61428	47.53	-0.2	0.0	4.3	0	0	-4	-1	-34	-303
C5r	5.9886	-38.05339	83.29	-2.0	1.2	4.4	0	0	0	74	-57	-4
H5r	0.9776	-0.61939	48.55	0.1	0.0	0.6	0	0	-1	-39	26	-45
C6r	5.9922	-38.06666	81.18	-1.3	1.4	3.7	0	0	2	47	47	95
H6r	0.9773	-0.62430	47.93	1.6	0.0	-4.9	-2	0	5	83	125	319
C4	5.9345	-38.05631	55.01	-5.7	-3.5	7.4	1	0	-1	106	-89	-60
H4a	0.9913	-0.62643	47.53	0.0	-0.2	-10.4	3	0	9	906	22	1021
H4e	0.9496	-0.61134	44.20	4.5	-0.1	-4.3	-6	0	4	-989	39	230
C5	5.7271	-37.91973	48.28	-13.7	-0.4	1.1	2	-1	2	-143	143	233
H5	0.9439	-0.61511	46.58	-0.7	-0.3	22.1	0	0	-21	-84	53	804
C6	5.9371	-38.01837	58.15	-2.2	-1.1	5.3	1	0	0	34	14	-18
H6a	0.9718	-0.62016	46.09	0.2	-0.2	-3.9	-1	0	4	-185	49	190
H6e	0.9924	-0.63026	47.76	0.9	0.0	-2.0	-1	0	2	-93	5	207
C7	5.9357	-38.01730	57.79	-4.3	-0.5	5.4	1	0	0	-208	-19	8
H7e	0.9873	-0.62862	47.08	-2.6	0.0	1.7	1	0	-1	-242	-98	-81
H7a	0.9759	-0.62193	46.10	1.4	-0.2	-0.9	-2	0	1	-57	37	42
N8	8.0193	-55.34322	58.49	40.2	1.4	2.3	-15	0	1	-419	5	-773
H8	0.4970	-0.40890	16.67	-26.1	-1.2	8.2	21	0	-9	3737	11	-4182
C8	5.6664	-37.86762	62.58	-19.5	-7.2	-1.1	4	-1	2	-90	15	-1242
Ha-(C8)	0.9204	-0.60002	41.40	-2.6	-0.8	21.8	0	1	-26	-310	85	-4270
Ha+(C8)	0.9519	-0.61006	46.49	2.9	-0.5	-9.7	-4	1	8	-209	-7	671
Hc(C8)	0.9632	-0.61873	44.03	1.6	-0.5	-12.9	-4	0	11	-809	21	550

Supplementary Table 2.4b Integrated properties of morphine in MC2.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.9849	-38.03163	83.32	-6.0	0.1	7.2	1	0	-9	82	7	-570
H1	0.9635	-0.61224	48.04	-1.7	0.0	15.8	1	0	-16	33	52	-1118
C2	5.9918	-38.03920	83.27	-7.5	-1.9	12.2	-4	0	-6	-243	182	-299
H2	0.9653	-0.61233	47.68	3.3	0.3	9.0	-3	0	-9	-129	21	-611
C3	5.4424	-37.73835	60.20	-39.6	-6.3	-28.5	15	-2	20	300	2	542
O3	9.1709	-75.89803	115.97	67.8	-0.4	-103.5	-8	1	50	400	-139	-5721
H(O3)	0.3676	-0.33393	18.42	4.0	2.4	38.3	0	0	-25	116	95	-2606
C4	5.5431	-37.88029	59.67	-32.9	-3.3	-23.8	10	0	18	194	-53	373
O	9.0185	-75.77631	104.90	65.9	5.4	-55.4	-19	1	45	336	-137	1448
C5	5.5590	-37.88635	41.04	-20.9	-0.5	-16.3	6	0	11	-185	255	138
H5	0.9741	-0.64529	41.20	-4.6	0.0	-1.8	1	0	2	-352	-18	84
C6	5.4387	-37.70116	45.42	-29.8	0.2	-6.4	10	1	7	38	119	150
H6	0.9883	-0.63100	48.77	0.2	0.0	8.5	-1	0	-8	-29	28	-487
O6	9.1139	-75.80635	125.35	31.6	-1.9	-17.3	-12	0	25	-161	41	3154
H(O6)	0.4027	-0.35611	21.26	-5.8	-0.1	12.9	6	0	-9	609	-32	-547
C7	6.0266	-38.07275	80.70	-4.0	-3.5	4.2	1	0	2	-24	-116	182
H7	0.9485	-0.60541	46.65	-6.3	0.1	8.1	7	0	-8	591	8	-567
C8	6.0211	-38.04632	83.39	-3.6	-0.9	6.6	-3	0	-6	-328	118	-416
H8	0.9539	-0.60695	47.60	-0.8	0.1	14.1	0	0	-14	-128	19	-946
C9	5.7576	-37.89352	48.35	0.9	0.7	4.6	-2	0	-1	-14	-12	58
H9	0.9661	-0.62552	45.96	-1.1	0.0	12.7	0	0	-11	-64	2	-770
C10	5.9281	-37.99971	58.46	-5.4	1.1	-0.2	0	0	1	41	56	161
H10e	0.9885	-0.62802	46.05	-1.1	-0.1	13.2	0	0	-12	-107	-30	-649
H10a	0.9605	-0.61338	46.80	-1.5	0.0	7.8	1	0	-7	8	-12	-507
C11	6.0155	-38.10452	69.36	-0.1	0.8	9.8	0	0	-8	411	-19	-388
C12	6.0404	-38.26392	59.41	1.4	0.4	9.3	-1	0	-6	341	-23	-223
C13	5.9564	-38.12322	41.06	5.8	0.4	5.3	-2	-1	-1	100	-70	6
C14	5.9472	-38.05330	49.17	-2.1	0.6	3.4	1	0	0	78	-44	52
H14	1.0223	-0.66180	42.31	0.5	-0.1	9.0	-1	0	-8	-8	-11	-428
C15	5.9255	-38.02397	55.80	0.6	0.2	2.4	-1	0	1	133	-19	-3
H15e	0.9621	-0.61534	45.23	1.2	-0.1	-9.7	0	0	8	266	12	361
H15a	1.0032	-0.63245	48.51	0.5	0.0	6.4	-1	0	-6	-59	-3	-439
C16	5.7277	-37.90148	53.80	0.1	0.9	5.4	-2	0	-2	-50	30	-12
H16e	0.9549	-0.61668	45.62	0.0	0.1	11.7	-1	0	-10	-16	15	-614
H16a	0.9481	-0.61775	42.12	-0.1	0.0	-2.0	1	0	1	293	56	9
N17	7.9556	-55.22459	58.91	-1.2	1.8	0.4	-2	0	3	-76	58	76
H17	0.5656	-0.45140	27.30	1.0	-0.1	6.7	0	0	-5	12	7	-317
C17	5.6765	-37.86635	62.89	-9.3	1.9	-1.2	4	0	2	142	-7	110
Ha+(C17)	0.9403	-0.60508	45.27	0.2	0.0	8.5	-1	0	-8	-99	43	-480
Ha-(C17)	0.9370	-0.60379	45.27	0.8	0.0	9.8	-1	0	-9	37	-10	-449
Hc(C17)	0.9403	-0.60757	43.70	0.8	0.0	-0.7	-1	0	0	56	-23	-24

Supplementary Table 2.5a Integrated properties of cocaine in MC3.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.7232	-37.91359	46.94	-0.2	1.4	7.8	0	0	-1	12	-21	24
H1	0.9606	-0.62205	45.57	0.2	0.0	5.1	0	0	-4	-25	-37	-225
C2	5.9344	-38.06655	48.15	2.7	1.4	10.0	0	0	0	47	22	-44
H2	0.9492	-0.61545	44.20	0.6	0.0	-0.4	0	0	1	37	-85	69
C1'	4.3859	-37.03066	34.16	2.5	1.7	10.3	-2	1	-1	27	79	-13
O1'	9.2068	-76.00291	123.16	-12.9	4.5	6.6	1	0	-3	-108	-69	-185
O2'	9.0948	-75.97425	101.39	4.5	3.4	17.4	-1	0	2	213	8	54
C3'	5.5426	-37.76361	62.98	-5.3	1.6	-0.9	2	0	2	85	34	43
Ht(C3')	0.9425	-0.60990	45.38	0.8	0.0	0.8	0	0	0	-17	-18	21
Hg+(C3')	0.9454	-0.60940	45.49	-0.4	0.0	5.3	0	0	-5	28	17	-344
Hg-(C3')	0.9491	-0.61091	46.25	1.6	0.0	0.7	-1	0	1	-211	0	34
C3	5.5022	-37.76036	40.75	-2.0	0.4	-0.5	5	0	3	260	-5	9
H3	0.9524	-0.62887	39.62	2.3	0.0	-1.9	0	0	3	482	13	110
O3	9.0886	-75.94502	95.50	-21.0	3.8	-0.4	3	0	-1	-274	-40	-74
O1"	9.2041	-76.01057	132.71	10.3	4.7	22.0	-1	1	3	764	57	2369
C1"	4.4768	-37.08138	39.99	20.1	-0.2	36.9	-10	0	-7	-168	-30	-140
C1r	5.9901	-38.09741	72.07	1.3	-6.5	-1.3	2	1	-2	116	158	-258
C2r	5.9874	-38.07493	79.81	3.9	-12.5	-14.5	0	-1	4	152	90	-1108
H2r	0.9525	-0.61149	46.37	0.0	0.5	-10.9	0	1	9	136	104	1644
C3r	5.9922	-38.05850	85.69	3.6	-10.0	-11.9	1	-1	9	106	220	2375
H3r	0.9751	-0.61813	52.05	1.3	0.5	-5.7	0	1	6	38	163	4042
C4r	5.9908	-38.05881	82.96	-2.5	-4.5	-3.7	1	0	3	126	129	264
H4r	0.9661	-0.61501	47.84	-0.3	0.2	2.3	0	0	-2	18	45	-87
C5r	5.9887	-38.05456	83.38	-3.0	-0.2	0.6	1	0	-1	117	27	-49
H5r	0.9712	-0.61692	48.05	-0.8	0.1	7.3	1	0	-8	-28	28	-537
C6r	5.9899	-38.06807	80.95	-3.8	-0.4	0.0	1	0	-1	-42	95	-84
H6r	0.9662	-0.61993	46.83	-1.4	0.1	8.2	1	0	-9	-15	14	-576
C4	5.9341	-38.05286	54.99	-0.4	0.9	7.2	0	0	0	22	-56	-26
H4a	0.9755	-0.62121	45.30	0.8	0.0	3.2	-1	0	-2	-166	22	-130
H4e	0.9564	-0.61327	45.24	0.3	0.0	-4.9	0	0	4	92	-11	224
C5	5.7214	-37.91132	48.05	-0.5	1.7	9.1	-1	0	-1	-35	29	19
H5	0.9612	-0.62174	45.66	0.1	0.0	3.7	0	0	-3	-3	10	-182
C6	5.9371	-38.01639	58.16	-0.7	1.8	7.2	1	0	0	38	26	-16
H6a	0.9753	-0.62123	46.46	0.0	0.1	-6.8	0	0	6	-12	79	355
H6e	0.9874	-0.62813	47.37	0.6	0.0	4.5	0	0	-3	-33	38	-268
C7	5.9356	-38.01506	58.03	-0.6	1.5	6.5	1	0	0	95	-71	-1
H7e	0.9832	-0.62658	47.19	-0.1	0.0	4.4	0	0	-4	-30	-4	-279
H7a	0.9799	-0.62301	46.43	1.4	0.0	-2.5	-1	0	4	78	40	240
N8	8.0330	-55.35540	59.71	0.3	2.4	12.0	-1	0	0	13	-4	19
H8	0.4850	-0.40130	17.14	0.1	0.1	0.8	0	0	0	75	-20	-15
C8	5.6646	-37.85620	64.04	-3.8	1.6	2.2	2	0	1	115	-37	74
Ha-(C8)	0.9417	-0.60538	45.63	0.7	0.0	4.3	0	0	-3	-28	-37	-191
Ha+(C8)	0.9425	-0.60554	45.82	0.3	0.0	4.6	0	0	-4	13	36	-268
Hc(C8)	0.9537	-0.61373	44.15	0.3	0.0	1.4	0	0	-1	-95	29	-70

Supplementary Table 2.5b Integrated properties of morphine in MC3.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.9942	-38.03371	84.03	1.3	-1.9	-3.1	0	0	1	-2	114	35
H1	0.9766	-0.61721	48.96	-0.4	0.1	-0.6	0	0	0	19	-15	65
C2	5.9782	-38.04031	83.84	0.0	-7.9	-10.1	-1	-1	1	116	-52	1108
H2	0.9461	-0.60523	47.53	0.9	0.2	-2.6	0	1	3	-15	69	1194
C3	5.4242	-37.73089	60.16	-15.5	-3.7	-30.7	5	0	8	57	45	901
O3	9.1415	-75.88338	123.31	16.6	0.5	-3.9	-4	1	11	-14	-228	1486
H(O3)	0.3847	-0.34560	20.45	-0.9	1.1	-0.1	1	0	0	-41	19	396
C4	5.5620	-37.89138	60.77	-2.1	0.3	-3.2	-2	-1	1	-89	-43	495
O	9.0232	-75.77617	108.32	-9.1	4.4	-9.8	0	0	1	-140	-54	1997
C5	5.5690	-37.89355	41.55	-2.0	-0.7	-3.8	-2	0	0	-200	-7	27
H5	0.9804	-0.64789	43.23	-2.3	0.0	-13.8	0	0	10	-282	27	2114
C6	5.4380	-37.70175	45.50	-7.6	0.3	-11.5	5	0	2	235	-31	59
H6	0.9897	-0.63024	49.06	0.8	0.0	7.3	-1	0	-6	138	-11	-384
O6	9.1042	-75.80626	124.95	11.8	0.7	4.0	-4	0	6	43	-41	2309
H(O6)	0.4041	-0.35801	21.14	-1.2	-0.2	-1.3	0	0	0	-48	7	10
C7	6.0105	-38.06971	79.91	-0.2	-4.2	-7.4	0	0	2	85	-12	93
H7	0.9269	-0.59725	45.01	-0.2	0.1	1.0	1	0	-1	125	8	-82
C8	6.0265	-38.04750	83.73	-2.0	-1.0	-4.2	0	0	-1	-47	-4	-39
H8	0.9609	-0.60967	48.05	-0.4	0.1	4.1	0	0	-4	-18	-17	-289
C9	5.7593	-37.89415	48.41	1.3	0.6	2.5	-1	0	-1	56	8	12
H9	0.9711	-0.62749	46.34	-0.2	0.0	4.8	0	0	-4	-78	74	-317
C10	5.9275	-37.99755	58.52	0.9	1.0	0.1	0	0	0	164	121	27
H10e	0.9957	-0.63081	46.47	-0.5	0.0	3.6	0	0	-4	-22	7	-195
H10a	0.9660	-0.61551	47.22	-0.4	0.0	-0.4	0	0	0	6	-30	-2
C11	6.0208	-38.10496	69.74	4.9	-0.1	4.5	-1	0	-2	187	-9	-114
C12	6.0419	-38.26446	59.31	5.8	0.9	5.7	1	0	-1	249	17	-27
C13	5.9589	-38.12404	41.17	4.9	1.2	6.1	0	0	-1	88	18	-11
C14	5.9471	-38.05348	49.17	-2.8	1.1	-3.3	0	0	0	-47	-24	33
H14	1.0261	-0.66347	42.42	-1.6	0.0	3.4	1	0	-4	-59	-7	-209
C15	5.9254	-38.02407	55.82	1.0	0.2	0.6	0	0	0	126	-39	8
H15e	0.9596	-0.61408	45.08	1.2	0.0	0.2	0	0	0	71	31	-5
H15a	1.0055	-0.63303	48.79	-0.5	0.1	3.7	1	0	-4	113	7	-282
C16	5.7292	-37.90267	53.89	0.3	1.8	1.9	-1	1	0	-50	86	-1
H16e	0.9595	-0.61852	45.87	0.0	0.0	5.8	0	0	-5	-5	-12	-301
H16a	0.9475	-0.61735	42.03	0.6	0.0	-2.0	0	0	2	222	-19	64
N17	7.9546	-55.22607	58.75	-1.4	1.7	-2.3	-1	0	1	-103	-11	43
H17	0.5676	-0.45243	27.37	0.1	0.0	4.1	0	0	-3	4	-14	-166
C17	5.6732	-37.86460	62.89	-2.1	1.5	-2.8	2	0	1	185	-75	83
Ha+(C17)	0.9439	-0.60644	45.57	0.6	0.0	4.0	0	0	-3	19	1	-202
Ha-(C17)	0.9409	-0.60545	45.37	0.5	0.0	5.5	0	0	-5	6	5	-286
Hc(C17)	0.9417	-0.60814	43.75	0.1	0.0	-2.0	0	0	2	-2	67	64

Supplementary Table 2.6a Integrated properties of cocaine in MC4.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.7230	-37.91346	46.79	2.9	1.4	3.8	-1	0	0	-161	18	3
H1	0.9641	-0.62372	45.71	1.9	0.0	-1.2	-2	0	1	-163	-10	25
C2	5.9330	-38.06945	47.87	-4.4	-1.2	8.0	-1	0	-1	-223	-67	35
H2	0.9451	-0.61490	43.72	-4.9	-0.1	6.0	2	0	-6	-187	47	-326
C1'	4.3881	-37.03196	34.10	5.2	-9.2	10.7	-2	0	2	165	-37	-93
O1'	9.2335	-76.00363	122.18	49.0	-1.1	-43.2	-1	0	25	2900	-61	-4161
O2'	9.0927	-75.98281	100.41	-24.8	-0.2	20.3	6	0	-8	-360	49	-413
C3'	5.5326	-37.75788	62.75	8.1	0.2	5.9	-5	0	-1	35	-57	-50
Ht(C3')	0.9371	-0.60768	45.05	-3.6	0.0	10.2	3	0	-9	156	74	-578
Hg+(C3')	0.9571	-0.61425	46.21	0.2	0.0	-7.5	0	0	7	-30	22	434
Hg-(C3')	0.9572	-0.61384	47.05	0.0	0.0	-6.9	1	0	6	221	21	403
C3	5.4906	-37.75478	40.37	9.0	0.5	4.5	-4	0	0	-126	-13	29
H3	0.9493	-0.62815	39.33	-6.5	-0.1	6.6	6	0	-5	483	37	-224
O3	9.0862	-75.93626	95.98	16.2	2.2	4.0	-4	0	3	-17	1	124
O1''	9.1989	-76.01813	128.65	-13.3	2.1	13.4	2	0	-4	-630	9	-243
C1''	4.4985	-37.09832	40.37	-9.0	-0.5	2.0	4	0	2	38	-30	31
C1r	5.9904	-38.09499	72.04	-0.6	1.1	4.7	-1	0	1	-5	-39	36
C2r	5.9827	-38.06744	80.61	-1.1	1.2	5.0	0	0	-1	63	-58	-89
H2r	0.9399	-0.60628	44.38	-0.7	0.0	3.4	1	0	-3	58	56	-221
C3r	5.9817	-38.05184	82.99	-1.5	1.3	5.8	0	0	-2	140	-60	-68
H3r	0.9629	-0.61385	47.44	-0.2	0.0	5.7	0	0	-5	-13	-3	-350
C4r	5.9859	-38.05532	82.45	-1.1	1.2	5.3	0	0	-1	67	-34	-35
H4r	0.9636	-0.61432	47.55	0.0	0.0	4.1	0	0	-4	-20	-43	-249
C5r	5.9892	-38.05316	83.41	-0.5	0.8	4.0	0	0	1	102	-68	101
H5r	0.9796	-0.62014	48.70	0.5	0.0	-1.7	0	0	2	-53	-23	162
C6r	5.9926	-38.06643	81.25	0.0	0.8	3.5	0	0	3	97	-5	162
H6r	0.9790	-0.62474	47.83	2.8	0.0	-7.1	-2	0	7	26	-61	458
C4	5.9357	-38.05599	55.12	-4.4	-1.0	4.4	1	1	0	-16	113	-31
H4a	0.9849	-0.62439	46.97	-0.7	-0.2	-4.3	2	0	4	566	-87	906
H4e	0.9447	-0.60906	43.92	4.2	0.0	2.0	-6	0	-2	-927	11	-81
C5	5.7245	-37.91540	48.11	-9.6	0.7	7.2	2	1	-1	-29	36	61
H5	0.9662	-0.62400	46.11	-0.4	-0.1	-1.7	0	0	2	78	-11	239
C6	5.9371	-38.01748	58.13	-1.1	1.1	4.3	0	0	0	-66	53	25
H6a	0.9653	-0.61732	45.75	0.7	-0.2	3.0	-1	0	-3	-138	24	-172
H6e	0.9890	-0.62898	47.39	0.1	0.0	2.2	0	0	-2	-138	31	-137
C7	5.9349	-38.01628	57.83	-2.6	0.6	5.2	1	-1	0	-102	-79	8
H7e	0.9843	-0.62726	47.13	-1.5	0.0	4.1	1	0	-4	-106	-35	-235
H7a	0.9730	-0.62054	45.88	0.8	-0.1	3.3	-1	0	-3	22	-25	-195
N8	8.0222	-55.34807	59.04	20.9	-0.4	10.9	-9	-1	-2	-151	-93	-396
H8	0.4945	-0.40789	16.72	-15.0	-0.8	-0.7	12	0	-2	2045	0	-2418
C8	5.6582	-37.85736	63.58	-11.6	-0.6	11.4	2	-1	-4	-6	-12	-296
Ha-(C8)	0.9470	-0.60865	47.25	-2.2	-0.3	-1.8	0	0	1	-134	24	1473
Ha+(C8)	0.9492	-0.60863	46.31	1.0	-0.2	-4.3	-2	0	4	-191	29	428
Hc(C8)	0.9531	-0.61400	43.82	1.0	-0.2	0.0	-2	0	0	-398	-54	-3

Supplementary Table 2.6b Integrated properties of morphine in MC4.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.9893	-38.03367	83.62	-6.9	0.3	3.5	0	0	-5	-24	87	-329
H1	0.9689	-0.61438	48.39	-0.8	0.0	7.7	0	0	-8	31	39	-573
C2	5.9830	-38.03987	82.94	-3.3	-4.7	-0.9	-2	0	6	-139	2	417
H2	0.9698	-0.61489	49.06	0.1	0.0	-28.0	0	0	26	8	10	2754
C3	5.4499	-37.74684	60.30	-26.2	-14.0	-31.7	18	-2	21	591	-45	583
O3	9.1743	-75.88281	122.61	83.1	-4.2	-82.5	-11	1	52	502	-235	361
H(O3)	0.3648	-0.33285	17.68	1.8	0.7	31.0	1	0	-20	158	75	-2622
C4	5.5463	-37.87855	59.94	19.4	-2.4	13.4	-12	0	-7	-186	23	-284
O	9.0212	-75.77324	106.69	-3.6	4.0	-2.2	-3	0	3	106	-69	142
C5	5.5817	-37.89876	41.94	-10.5	0.8	-8.0	6	0	4	131	17	60
H5	0.9718	-0.64395	41.20	-0.4	0.0	-3.0	-1	0	3	-271	-65	151
C6	5.4319	-37.69675	45.43	0.0	1.4	0.1	0	0	1	94	40	58
H6	0.9917	-0.63147	49.03	-1.2	0.0	5.4	1	0	-5	16	39	-340
O6	9.1009	-75.80912	122.64	-8.9	2.7	2.5	0	0	-1	47	-28	-26
H(O6)	0.4069	-0.35990	21.33	-0.6	-0.1	-5.7	-1	0	4	-134	14	278
C7	6.0091	-38.06957	79.66	-8.0	-0.1	1.0	1	0	0	26	-81	-31
H7	0.9217	-0.59524	44.66	-0.1	0.0	6.4	0	0	-6	80	-23	-354
C8	6.0262	-38.04816	83.63	-7.4	0.7	0.8	0	0	-1	-87	29	-121
H8	0.9569	-0.60814	47.79	-0.3	0.0	8.4	0	0	-8	-40	18	-581
C9	5.7579	-37.89442	48.29	-1.6	1.2	2.4	-2	0	0	6	-121	66
H9	0.9670	-0.62592	46.09	-1.0	0.0	9.9	0	0	-9	-42	38	-572
C10	5.9281	-37.99940	58.44	-4.9	1.2	-1.0	1	0	1	88	7	129
H10e	0.9917	-0.62927	46.20	-1.5	0.0	9.1	1	0	-8	-16	-60	-417
H10a	0.9606	-0.61346	46.78	-1.2	0.0	6.1	0	0	-5	-17	-54	-384
C11	6.0164	-38.10542	69.32	-5.3	1.2	7.4	0	0	-7	6	-25	-337
C12	6.0384	-38.26248	59.37	4.8	1.6	4.6	1	0	-5	409	17	-130
C13	5.9572	-38.12369	41.08	4.2	1.2	1.8	-1	-1	-1	76	-61	-11
C14	5.9467	-38.05358	49.19	-5.8	1.2	1.1	0	0	0	-89	44	39
H14	1.0247	-0.66322	42.28	-2.8	0.0	6.9	1	0	-6	-83	-12	-321
C15	5.9258	-38.02340	55.80	0.7	0.6	1.1	0	0	0	92	-9	-3
H15e	0.9637	-0.61589	45.33	0.3	0.0	-4.9	0	0	4	219	-2	141
H15a	1.0034	-0.63256	48.59	-2.3	0.1	7.2	1	0	-7	14	53	-423
C16	5.7269	-37.90115	53.81	1.9	1.3	2.7	-2	0	-1	-82	58	-20
H16e	0.9571	-0.61765	45.73	-0.3	0.0	8.4	0	0	-7	-22	6	-443
H16a	0.9499	-0.61847	42.20	0.5	0.0	-5.5	0	0	4	293	-17	171
N17	7.9565	-55.22760	58.93	-6.9	2.1	-1.6	0	0	2	-53	79	82
H17	0.5656	-0.45128	27.25	0.6	0.0	6.5	0	0	-5	24	-43	-283
C17	5.6752	-37.86601	62.89	-6.3	1.4	-1.6	3	0	1	245	-124	63
Ha+(C17)	0.9408	-0.60518	45.39	0.7	0.0	6.6	-1	0	-6	-26	28	-373
Ha-(C17)	0.9387	-0.60457	45.30	0.4	0.0	7.4	0	0	-7	-7	-6	-334
Hc(C17)	0.9420	-0.60841	43.70	0.2	0.0	-2.9	0	0	2	-53	25	105

Supplementary Table 2.7a Integrated properties of ecgonine methyl ester in ME1.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b{}^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b{}^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b{}^{CP}v(\Omega)\cdot10^3$
C1	5.7228	-37.91353	46.97	-2.3	0.2	3.3	0	0	0	3	-15	26
H1	0.9633	-0.62327	45.76	-0.9	0.0	1.4	1	0	-1	32	-29	-25
C2	5.9491	-38.07862	48.57	3.9	-0.6	3.3	-3	0	-2	-34	-35	-134
H2	0.9668	-0.62239	45.40	1.1	0.0	-4.8	-1	0	4	-57	-19	270
C1'	4.3856	-37.03055	33.86	-6.8	-0.4	3.2	3	0	0	65	-28	-16
O1'	9.2078	-76.00281	123.24	-13.3	1.8	10.5	1	0	-2	-355	-5	-94
O2'	9.0985	-75.97140	100.85	16.6	1.1	-2.6	-5	0	5	232	3	245
C3'	5.5401	-37.76214	62.63	-1.5	0.0	4.8	-1	0	-1	-103	-49	18
Ht(C3')	0.9493	-0.61284	45.78	0.0	0.0	-6.2	0	0	5	81	-35	330
Hg+(C3')	0.9456	-0.60980	45.33	-2.3	0.0	6.1	2	0	-5	-22	76	-335
Hg-(C3')	0.9461	-0.60959	45.64	-0.1	0.0	-2.3	0	0	2	35	-3	148
C3	5.4257	-37.69087	41.31	11.3	-2.2	11.6	-6	0	-5	-95	76	-352
H3	1.0018	-0.64644	45.79	-1.9	0.0	2.1	1	0	-1	25	35	323
O3	9.1400	-75.83533	122.19	7.7	-1.2	-42.0	3	-1	29	619	-245	2691
H(O3)	0.3768	-0.34186	16.09	5.5	-0.6	31.5	-1	1	-24	22	117	-5022
C4	5.9276	-38.04992	54.62	-2.2	-0.7	2.7	1	0	0	0	-42	-69
H4a	0.9716	-0.61973	45.02	-0.1	-0.1	-3.4	0	0	3	-116	57	204
H4e	0.9763	-0.61991	47.64	-2.3	0.0	-7.2	2	0	7	140	24	523
C5	5.7222	-37.91142	48.09	1.2	0.0	3.6	0	0	1	115	-12	155
H5	0.9647	-0.62342	45.91	0.1	0.1	-0.5	0	0	1	50	-35	98
C6	5.9365	-38.01609	58.21	-0.4	-0.1	2.2	0	0	0	-2	153	-67
H6a	0.9808	-0.62326	46.90	-0.4	0.1	-1.3	1	0	1	-27	29	171
H6e	0.9888	-0.62876	47.45	0.2	0.0	1.0	0	0	-1	-4	-22	-67
C7	5.9354	-38.01438	58.17	-2.8	-0.2	4.3	0	0	0	-15	-9	73
H7e	0.9845	-0.62709	47.34	-0.5	0.0	2.3	0	0	-2	-28	26	-86
H7a	0.9863	-0.62575	46.93	-0.2	0.1	-4.8	0	0	4	22	2	275
N8	8.0340	-55.35756	59.60	-5.9	1.0	6.4	0	0	0	13	-63	-4
H8	0.4840	-0.40072	17.05	-0.8	0.0	-0.8	0	0	0	15	3	-47
C8	5.6636	-37.85499	64.02	-2.7	-0.2	3.0	1	0	1	61	-75	37
Ha-(C8)	0.9432	-0.60608	45.69	-0.1	0.0	1.7	0	0	-1	-13	-12	-110
Ha+(C8)	0.9428	-0.60576	45.79	-0.2	0.0	2.5	0	0	-2	-25	25	-167
Hc(C8)	0.9549	-0.61393	44.34	1.0	0.1	1.2	0	0	-1	90	27	-53

Supplementary Table 2.7b Integrated properties of morphine in ME1.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.9839	-38.03136	83.35	-7.7	0.2	9.5	1	0	-9	23	-16	-520
H1	0.9633	-0.61208	48.01	-1.6	0.0	14.9	1	0	-15	54	8	-1032
C2	5.9916	-38.03912	82.89	-10.6	-1.3	14.8	-3	0	-6	-320	5	-298
H2	0.9691	-0.61379	47.81	1.3	0.1	6.1	-1	0	-6	-78	-40	-359
C3	5.4632	-37.74691	60.63	-59.1	-3.9	-31.6	29	-1	26	671	-6	598
O3	9.1498	-75.86780	118.36	104.7	2.2	-64.6	-20	1	41	372	62	-3536
H(O3)	0.3851	-0.34557	20.38	-4.9	1.7	16.2	3	0	-10	169	3	-563
C4	5.5206	-37.86296	59.15	1.2	-3.6	-3.0	-6	0	5	-129	-72	-15
O	9.0090	-75.78027	106.60	21.6	1.8	-17.6	-10	1	22	28	-18	2708
C5	5.5674	-37.88759	41.72	-9.5	-0.6	-9.0	3	0	8	97	-82	184
H5	0.9938	-0.65219	42.58	-1.1	-0.1	1.6	0	0	-1	-36	-12	-63
C6	5.4198	-37.69262	44.64	-19.9	0.1	-2.0	6	0	5	109	26	137
H6	0.9687	-0.62516	47.18	4.0	-0.1	1.8	-3	0	-2	-3	1	-120
O6	9.0978	-75.80231	122.39	16.3	0.2	-5.3	-9	0	10	-304	68	748
H(O6)	0.4173	-0.36327	22.66	-4.6	-0.1	-0.7	3	0	1	346	4	20
C7	6.0343	-38.07502	81.12	-1.1	-0.5	5.1	3	0	2	210	-37	50
H7	0.9420	-0.60244	46.30	-6.1	0.0	6.4	6	0	-6	384	24	-382
C8	6.0257	-38.04678	83.46	-3.6	-0.4	5.8	-3	0	-5	-318	-106	-261
H8	0.9553	-0.60753	47.70	-0.5	0.0	11.7	0	0	-11	-68	-42	-799
C9	5.7584	-37.89275	48.49	2.0	0.0	4.4	-2	0	0	111	-78	177
H9	0.9664	-0.62553	46.02	-0.3	-0.1	10.7	0	0	-9	41	18	-693
C10	5.9278	-37.99964	58.35	-4.7	0.2	-0.4	1	0	1	135	7	98
H10e	0.9897	-0.62847	46.12	-1.8	0.0	11.8	0	0	-10	-35	-30	-536
H10a	0.9599	-0.61309	46.74	-1.1	0.0	8.5	0	0	-7	-82	61	-557
C11	6.0153	-38.10618	69.07	-4.6	0.1	8.7	0	0	-7	52	71	-405
C12	6.0416	-38.26381	59.44	-1.6	0.7	8.6	0	0	-6	227	21	-201
C13	5.9579	-38.12326	41.21	5.1	1.0	5.7	0	1	0	160	115	42
C14	5.9473	-38.05350	49.27	-5.6	0.2	3.2	1	0	-1	128	-44	-17
H14	1.0228	-0.66293	42.03	-2.9	0.0	7.0	0	0	-6	-248	-11	-284
C15	5.9257	-38.02286	55.83	3.4	-0.5	2.6	-1	0	1	101	-67	53
H15e	0.9597	-0.61424	45.12	0.6	-0.1	-7.0	0	0	6	267	-49	274
H15a	1.0032	-0.63244	48.57	-0.7	0.0	3.9	0	0	-4	67	32	-250
C16	5.7288	-37.90119	53.91	0.7	0.8	5.0	-1	0	-2	18	-6	14
H16e	0.9564	-0.61733	45.64	-0.1	0.0	8.4	0	0	-7	-6	-12	-470
H16a	0.9484	-0.61792	42.07	0.4	0.0	-2.2	0	0	1	145	19	50
N17	7.9557	-55.22566	58.79	-1.9	0.9	0.5	-1	0	2	-72	77	6
H17	0.5661	-0.45164	27.26	0.3	0.0	5.2	0	0	-4	-29	10	-265
C17	5.6753	-37.86521	63.04	-6.5	1.0	-0.3	3	0	2	10	142	89
Ha+(C17)	0.9405	-0.60501	45.36	0.6	0.0	7.6	-1	0	-7	71	-31	-446
Ha-(C17)	0.9381	-0.60431	45.21	0.7	0.0	7.5	-1	0	-7	-13	-44	-383
Hc(C17)	0.9409	-0.60785	43.65	0.6	0.0	-0.6	0	0	0	79	-55	-5

Supplementary Table 2.8a Integrated properties of ecgonine methyl ester in ME2.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.7237	-37.91470	46.88	-1.9	-0.1	3.8	0	-1	0	-44	-52	23
H1	0.9622	-0.62283	45.63	-0.9	0.0	2.4	1	0	-2	18	-14	-129
C2	5.9387	-38.07265	48.15	-5.7	0.1	3.8	3	0	0	104	23	-36
H2	0.9560	-0.61850	44.62	-6.5	0.0	-3.4	6	0	3	280	-16	150
C1'	4.3837	-37.02913	33.80	-14.5	-0.1	2.9	5	0	1	245	-14	-46
O1'	9.2090	-76.00081	123.39	-13.1	1.9	9.5	0	0	-1	-62	14	-64
O2'	9.0944	-75.97570	100.32	13.4	0.9	3.6	-1	0	3	649	-31	96
C3'	5.5368	-37.76021	62.53	-2.5	-0.4	7.1	-1	0	-1	-44	-65	-39
Ht(C3')	0.9465	-0.61170	45.61	-0.9	0.0	-3.9	1	0	3	45	-13	228
Hg+(C3')	0.9472	-0.61031	45.53	-2.1	0.1	7.2	2	0	-6	98	-9	-398
Hg-(C3')	0.9512	-0.61174	45.94	1.2	0.0	-8.1	-1	0	7	-81	16	458
C3	5.4299	-37.69244	41.53	17.0	-1.4	12.8	-5	-1	-5	74	14	-142
H3	1.0100	-0.65015	46.01	-2.2	0.0	-5.8	2	0	6	161	47	560
O3	9.1536	-75.83650	123.66	23.3	-2.7	-58.6	4	0	39	953	-188	3143
H(O3)	0.3708	-0.33730	14.87	10.9	-0.5	35.8	-4	1	-25	-208	119	-5985
C4	5.9358	-38.05315	55.23	5.1	-0.5	4.7	-7	0	-1	-353	72	-57
H4a	0.9722	-0.61982	45.12	2.4	-0.1	-3.9	-3	0	4	-182	-5	253
H4e	0.9853	-0.62327	48.35	4.7	0.0	-4.7	-5	0	4	-447	-32	396
C5	5.7223	-37.91139	48.16	-6.8	0.0	4.1	1	0	0	73	42	33
H5	0.9635	-0.62286	45.80	0.1	0.0	1.4	0	0	-1	-27	20	-81
C6	5.9360	-38.01589	58.12	-5.0	0.2	5.1	0	0	0	76	-28	-13
H6a	0.9854	-0.62530	47.15	-0.6	0.1	-4.2	0	0	4	50	2	300
H6e	0.9860	-0.62765	47.32	-0.1	0.0	4.2	0	0	-4	26	-22	-253
C7	5.9350	-38.01490	58.09	-4.8	0.0	5.0	0	0	0	-24	-16	-4
H7e	0.9824	-0.62634	47.14	-0.9	-0.1	4.6	0	0	-4	-23	6	-299
H7a	0.9840	-0.62464	46.83	-1.6	0.1	-3.2	2	0	3	157	62	209
N8	8.0334	-55.35579	59.65	0.7	0.8	7.8	-2	0	0	43	-76	-12
H8	0.4849	-0.40112	17.10	-3.1	0.0	-2.4	2	0	1	267	-22	23
C8	5.6634	-37.85515	64.03	-4.5	-0.3	3.1	2	0	1	95	-65	45
Ha-(C8)	0.9427	-0.60588	45.63	0.5	0.0	2.2	-1	0	-2	-55	-67	-109
Ha+(C8)	0.9427	-0.60573	45.83	-0.4	0.0	2.8	0	0	-3	2	37	-168
Hc(C8)	0.9538	-0.61364	44.28	0.4	0.0	2.5	0	0	-2	21	-28	-105

Supplementary Table 2.8b Integrated properties of morphine in ME2.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.9894	-38.03287	83.52	-5.8	0.4	4.5	0	0	-4	-20	-78	-277
H1	0.9673	-0.61371	48.23	-0.3	0.0	8.9	0	0	-9	13	-41	-631
C2	5.9757	-38.03671	82.55	-5.3	0.7	4.0	0	0	-3	61	-9	-157
H2	0.9350	-0.60094	45.72	0.2	0.0	8.4	0	0	-8	-71	6	-494
C3	5.4071	-37.71643	59.03	1.7	-0.1	5.5	-3	0	-2	-58	-9	-72
O3	9.1299	-75.88329	121.74	-12.8	1.2	8.2	1	0	-4	-96	-20	-209
H(O3)	0.3859	-0.34702	20.17	0.3	0.1	-4.3	-1	0	3	-37	5	124
C4	5.5833	-37.89997	60.92	-18.7	0.0	-7.1	12	0	7	352	20	158
O	9.0239	-75.77005	106.80	3.9	1.3	0.5	-1	0	3	182	-58	147
C5	5.5567	-37.88466	41.15	8.0	0.1	11.7	-12	0	-2	-508	-61	-21
H5	0.9731	-0.64388	41.43	-0.2	0.0	-3.1	0	0	2	24	-54	74
C6	5.4783	-37.72751	45.97	-56.8	-1.5	-20.7	31	-1	18	434	-65	361
H6	0.9825	-0.62877	48.47	-0.9	0.0	12.2	-2	0	-12	-176	-11	-651
O6	9.1226	-75.79876	117.76	97.7	-2.5	-71.9	-22	1	41	564	-282	-5154
H(O6)	0.3963	-0.35297	20.82	-3.0	1.0	13.9	2	0	-9	244	18	-634
C7	6.0145	-38.06460	80.41	11.7	-3.4	-2.4	-3	-1	9	209	-25	493
H7	0.9367	-0.60214	46.09	1.7	-0.4	-13.1	0	1	9	297	40	804
C8	6.0164	-38.04213	82.95	-1.6	-1.5	13.0	0	0	-11	-66	-24	-768
H8	0.9579	-0.60884	47.87	-1.2	0.0	7.4	1	0	-8	13	-69	-473
C9	5.7579	-37.89146	48.41	2.7	0.5	6.6	-1	0	-2	63	-27	29
H9	0.9707	-0.62728	46.31	0.5	0.0	4.9	-1	0	-4	-51	-19	-286
C10	5.9264	-37.99792	58.34	-3.7	0.9	2.0	0	0	0	-49	128	47
H10e	0.9913	-0.62931	46.11	-1.7	0.0	9.2	0	0	-8	-137	57	-501
H10a	0.9652	-0.61512	47.15	0.5	0.0	0.1	0	0	0	-56	7	-54
C11	6.0199	-38.10581	69.50	-3.4	0.0	5.7	-1	0	-3	-121	42	-110
C12	6.0408	-38.26531	59.08	-0.2	0.6	3.2	-1	0	0	-7	7	9
C13	5.9602	-38.12569	41.11	-5.1	0.3	6.7	0	1	0	-1	13	18
C14	5.9478	-38.05258	49.30	-0.5	-0.9	0.6	1	-1	1	158	-100	47
H14	1.0251	-0.66289	42.43	-0.4	0.0	5.3	-1	0	-4	-70	23	-217
C15	5.9265	-38.02404	55.89	-0.7	0.0	1.3	0	0	1	33	96	44
H15e	0.9570	-0.61327	44.84	-0.8	0.0	3.1	1	0	-3	74	18	-227
H15a	1.0097	-0.63481	48.97	1.2	0.0	-2.1	-1	0	2	-72	5	79
C16	5.7293	-37.90288	53.89	-2.4	0.6	3.1	0	0	0	21	-52	67
H16e	0.9574	-0.61777	45.70	-0.6	-0.1	8.5	0	0	-7	12	15	-502
H16a	0.9419	-0.61522	41.61	-0.5	0.0	4.1	0	0	-4	112	-18	-233
N17	7.9539	-55.22291	58.78	2.8	0.4	2.6	-2	0	1	28	-68	7
H17	0.5693	-0.45349	27.51	1.0	0.0	0.4	0	0	-1	21	-12	-55
C17	5.6754	-37.86578	62.88	-6.2	0.3	0.1	3	0	2	139	-50	90
Ha+(C17)	0.9429	-0.60600	45.51	0.7	0.0	4.5	-1	0	-4	1	-9	-242
Ha-(C17)	0.9390	-0.60478	45.27	0.0	0.0	7.2	0	0	-6	26	-9	-394
Hc(C17)	0.9371	-0.60633	43.38	-0.1	0.0	2.8	0	0	-3	-75	37	-183

Supplementary Table 2.9a Integrated properties of ecgonine methyl ester in ME3.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.7203	-37.91056	46.87	5.8	1.4	1.9	-1	-1	-1	53	-60	-79
H1	0.9641	-0.62351	45.77	1.5	0.0	-1.6	-1	0	2	-100	54	34
C2	5.9508	-38.08031	48.62	-5.6	-0.1	7.9	-2	0	-1	-242	20	73
H2	0.9593	-0.62033	44.59	-4.5	-0.2	6.5	1	0	-6	-328	22	-313
C1'	4.3814	-37.02633	33.65	5.7	-7.8	9.1	-4	0	2	-137	-4	-43
O1'	9.2354	-76.00147	122.08	51.9	-1.0	-48.5	-1	0	28	2881	-166	-4326
O2'	9.0975	-75.98040	99.79	-25.3	1.9	15.5	6	0	-7	59	-79	-566
C3'	5.5378	-37.75972	62.62	6.2	1.7	1.7	-4	0	0	-13	18	-165
Ht(C3')	0.9350	-0.60689	44.93	-3.0	0.1	12.4	2	0	-11	155	6	-647
Hg+(C3')	0.9555	-0.61363	46.14	-0.1	0.0	-6.2	1	0	5	137	-2	390
Hg-(C3')	0.9502	-0.61103	46.00	0.0	0.0	-6.2	1	0	6	232	65	241
C3	5.4383	-37.69836	41.81	-3.7	1.1	3.9	1	0	0	34	-8	100
H3	0.9959	-0.64443	45.27	-2.1	0.0	7.6	1	0	-6	162	56	-351
O3	9.1111	-75.81930	119.05	0.7	4.3	0.9	-1	0	4	-156	19	56
H(O3)	0.3969	-0.35357	20.74	0.8	-0.1	4.9	-1	0	-3	-52	-21	-181
C4	5.9260	-38.04971	54.74	-3.1	-0.8	4.3	0	0	-1	42	-27	-6
H4a	0.9762	-0.62137	45.90	1.4	-0.1	-9.2	-1	0	8	51	23	952
H4e	0.9673	-0.61634	46.99	0.4	-0.1	-0.4	0	0	0	17	45	-18
C5	5.7221	-37.91335	48.02	-8.7	1.0	7.4	2	0	-1	125	47	23
H5	0.9645	-0.62347	45.96	-1.1	-0.1	0.7	0	0	0	-39	11	192
C6	5.9367	-38.01607	58.10	-2.1	0.2	3.6	0	0	0	19	-53	20
H6a	0.9772	-0.62196	46.52	1.8	-0.1	0.2	-1	0	0	-87	48	-164
H6e	0.9878	-0.62852	47.24	-0.7	0.0	2.5	0	0	-2	-179	34	-159
C7	5.9356	-38.01448	58.05	-4.2	1.0	4.2	0	0	0	-157	58	32
H7e	0.9838	-0.62698	47.12	-1.2	0.0	3.3	0	0	-3	-71	9	-243
H7a	0.9787	-0.62278	46.38	1.6	-0.1	1.4	-2	0	-2	-123	54	-184
N8	8.0227	-55.34572	58.90	16.3	2.6	13.8	-9	0	-2	-211	22	-564
H8	0.4938	-0.40766	16.42	-18.1	-1.0	-0.7	13	0	-3	2168	11	-2838
C8	5.6661	-37.86146	63.34	-11.4	-3.1	-2.3	3	-2	2	40	-136	-554
Ha-(C8)	0.9183	-0.59701	43.89	1.2	-0.7	24.9	-2	1	-25	-165	61	-1829
Ha+(C8)	0.9538	-0.61058	46.64	0.1	-0.4	-10.1	-1	1	9	-144	-35	863
Hc(C8)	0.9605	-0.61724	44.11	2.2	-0.4	-8.3	-3	0	7	-412	-1	243

Supplementary Table 2.9b Integrated properties of morphine in ME3.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.9856	-38.03097	83.39	-4.8	0.5	7.3	1	0	-8	7	11	-483
H1	0.9647	-0.61262	48.07	-1.9	0.0	13.8	1	0	-14	54	5	-954
C2	5.9944	-38.03939	83.32	-5.6	-3.1	11.0	-3	0	-4	-89	142	-253
H2	0.9694	-0.61398	47.92	1.5	0.2	5.3	-2	0	-5	-44	16	-343
C3	5.4436	-37.73944	60.23	-33.3	-14.4	-27.3	15	-1	20	308	7	542
O3	9.1739	-75.89260	119.47	68.8	-4.5	-86.9	-8	1	54	450	-182	-2263
H(O3)	0.3699	-0.33543	18.15	3.2	2.0	34.4	0	0	-23	190	72	-2883
C4	5.5367	-37.87345	59.57	-18.1	-2.5	-12.0	2	0	12	-57	-14	290
O	9.0161	-75.77395	106.02	54.7	5.1	-38.0	-18	1	37	12	-99	2221
C5	5.5704	-37.88959	41.73	-13.1	0.1	-11.3	5	-1	9	162	-53	105
H5	0.9937	-0.65210	42.61	-0.2	-0.1	1.0	-1	0	-1	-69	-19	-7
C6	5.4204	-37.69319	44.67	-23.5	0.7	-0.5	8	0	5	291	-146	167
H6	0.9664	-0.62404	47.04	4.2	-0.1	4.5	-2	0	-4	93	26	-364
O6	9.0956	-75.80051	122.15	16.3	2.5	-3.0	-9	0	9	-253	-76	593
H(O6)	0.4176	-0.36348	22.68	-4.8	-0.2	-1.0	3	0	1	312	-3	82
C7	6.0345	-38.07444	81.17	-0.1	-0.8	5.9	3	0	1	154	-73	181
H7	0.9422	-0.60252	46.30	-8.9	0.0	8.9	8	0	-8	547	21	-545
C8	6.0249	-38.04618	83.44	-3.8	0.5	6.7	-4	0	-4	-378	0	-328
H8	0.9545	-0.60726	47.68	-0.6	0.1	12.5	-1	0	-12	-179	77	-834
C9	5.7578	-37.89239	48.46	1.2	1.3	4.9	-1	0	-1	165	-32	37
H9	0.9660	-0.62539	46.04	-1.2	-0.1	12.0	0	0	-10	10	3	-634
C10	5.9275	-37.99867	58.33	-4.5	0.9	1.4	1	0	1	159	-67	138
H10e	0.9898	-0.62846	46.18	-1.4	0.0	11.5	0	0	-10	-44	35	-545
H10a	0.9603	-0.61331	46.75	-1.3	0.0	8.1	1	0	-7	-35	17	-551
C11	6.0161	-38.10505	69.09	-3.6	0.2	10.6	1	-1	-7	443	-360	-353
C12	6.0412	-38.26355	59.42	-4.9	1.2	12.1	-1	0	-5	102	16	-94
C13	5.9569	-38.12243	41.16	5.9	1.4	6.6	1	0	-1	271	24	-23
C14	5.9474	-38.05351	49.35	-7.2	1.3	3.7	0	0	0	41	87	21
H14	1.0221	-0.66287	41.93	-2.2	0.0	6.5	0	0	-7	-180	28	-487
C15	5.9255	-38.02193	55.85	2.3	0.7	5.1	-1	0	0	111	0	2
H15e	0.9637	-0.61592	45.37	0.4	-0.1	-11.2	0	0	10	138	29	576
H15a	1.0014	-0.63175	48.46	-1.0	0.0	6.0	0	0	-6	164	-16	-411
C16	5.7277	-37.90048	53.87	0.4	1.7	6.3	-1	1	-3	-48	87	-59
H16e	0.9560	-0.61715	45.67	-0.9	0.0	9.6	0	0	-8	-19	66	-503
H16a	0.9491	-0.61814	42.13	0.8	0.0	-3.2	0	0	2	233	29	3
N17	7.9561	-55.22526	58.83	-2.8	2.6	0.6	-2	0	3	-112	127	31
H17	0.5656	-0.45135	27.24	-0.6	0.0	6.8	0	0	-5	-12	29	-321
C17	5.6756	-37.86496	62.96	-7.8	1.8	0.9	3	0	2	112	18	28
Ha+(C17)	0.9400	-0.60472	45.39	0.3	0.0	8.6	0	0	-8	75	-26	-414
Ha-(C17)	0.9377	-0.60416	45.31	0.4	0.0	8.1	0	0	-7	-36	33	-333
Hc(C17)	0.9412	-0.60796	43.68	0.9	0.0	-1.2	-1	0	1	53	77	-79

Supplementary Table 2.10a Integrated properties of ecgonine methyl ester in ME4.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b{}^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b{}^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b{}^{CP}v(\Omega)\cdot10^3$
C1	5.7245	-37.91291	47.08	-0.1	0.6	2.4	1	-1	2	1	-22	137
H1	0.9623	-0.62283	45.67	1.6	0.0	0.1	-1	0	0	-99	17	-25
C2	5.9508	-38.07932	48.64	-5.4	-0.5	10.7	-1	0	-1	-155	-27	57
H2	0.9575	-0.61929	44.56	-3.0	-0.1	7.5	1	0	-7	-231	-10	-406
C1'	4.3813	-37.02719	33.72	1.9	-11.7	14.9	-1	0	0	-8	-71	-40
O1'	9.2346	-76.00089	123.05	57.2	0.8	-54.1	-3	0	30	2068	-206	-2505
O2'	9.0963	-75.97919	99.83	-31.8	1.8	24.9	6	0	-8	-192	-81	-264
C3'	5.5391	-37.76265	63.07	0.6	-0.3	1.6	-2	0	-1	21	76	196
Ht(C3')	0.9376	-0.60804	45.10	-1.9	-0.1	8.4	1	0	-7	85	-13	-390
Hg+(C3')	0.9521	-0.61219	46.85	-0.1	0.0	-2.3	0	0	3	-11	32	1205
Hg-(C3')	0.9476	-0.61023	46.96	-0.1	0.0	-4.0	0	0	3	194	13	1295
C3	5.4398	-37.69931	41.75	-0.7	1.2	-1.6	1	0	2	130	-17	-37
H3	0.9945	-0.64396	45.16	-1.1	0.0	7.8	1	0	-7	163	1	-416
O3	9.1114	-75.81884	119.35	-1.6	2.2	6.6	-1	0	4	-265	15	463
H(O3)	0.3964	-0.35334	20.63	0.9	0.0	5.2	-1	0	-4	-50	-40	-284
C4	5.9265	-38.04946	54.70	-1.9	-0.6	3.5	0	0	0	7	-20	-16
H4a	0.9750	-0.62059	45.72	1.4	-0.1	-7.2	0	0	7	177	22	633
H4e	0.9646	-0.61533	46.77	-0.8	0.0	3.4	1	0	-3	29	27	-226
C5	5.7257	-37.91403	48.04	-5.7	1.0	2.6	3	0	2	222	-28	15
H5	0.9614	-0.62203	45.70	0.3	0.0	3.0	0	0	-2	-7	40	-128
C6	5.9360	-38.01599	58.14	-3.1	1.2	3.9	0	0	0	-15	-7	47
H6a	0.9753	-0.62136	46.32	0.3	-0.1	3.2	0	0	-3	-34	5	-365
H6e	0.9844	-0.62697	47.17	0.0	0.0	5.9	0	0	-5	-56	9	-316
C7	5.9353	-38.01467	58.01	-4.7	1.0	4.3	-1	0	0	-82	1	-30
H7e	0.9813	-0.62594	46.96	-0.7	0.0	5.5	0	0	-5	-49	-9	-411
H7a	0.9774	-0.62215	46.33	0.2	-0.1	4.5	-1	0	-4	-82	10	-238
N8	8.0238	-55.34685	59.61	16.4	1.3	11.9	-7	0	-3	9	-42	-2
H8	0.4977	-0.40974	19.29	-11.2	-0.1	-14.1	8	0	6	1317	4	895
C8	5.6642	-37.85638	64.13	-7.6	0.2	3.9	2	-1	1	13	-57	168
Ha-(C8)	0.9422	-0.60576	45.80	-0.2	-0.2	2.8	0	0	-2	-70	18	25
Ha+(C8)	0.9459	-0.60718	45.99	1.4	-0.1	-2.7	-1	0	2	-94	14	109
Hc(C8)	0.9504	-0.61242	43.85	1.3	-0.1	5.0	-1	0	-4	-171	35	-306

Supplementary Table 2.10b Integrated properties of morphine in ME4.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.9905	-38.03205	83.70	-3.6	0.8	3.2	0	0	-4	-45	65	-271
H1	0.9693	-0.61447	48.39	-0.7	0.0	7.4	0	0	-7	51	-48	-519
C2	5.9812	-38.03805	82.82	-0.8	-3.2	-0.4	-1	0	3	-18	45	110
H2	0.9546	-0.60872	46.96	0.1	0.0	-12.1	0	0	11	27	6	662
C3	5.4333	-37.73403	59.88	-16.2	-8.8	-14.1	11	-1	12	361	-50	369
O3	9.1685	-75.88360	125.13	56.8	-4.3	-57.6	-7	0	42	403	-189	2938
H(O3)	0.3673	-0.33498	16.73	2.6	0.1	22.6	0	1	-16	125	109	-3460
C4	5.5587	-37.88887	60.21	5.2	-3.4	3.5	-4	0	1	-99	12	4
O	9.0212	-75.77895	107.99	0.5	4.2	-11.7	-3	0	10	-10	-90	2485
C5	5.5653	-37.88679	41.65	-9.3	0.7	-6.3	-2	0	3	-263	61	-31
H5	0.9940	-0.65228	42.57	-1.1	-0.1	-0.7	0	0	1	-64	-24	28
C6	5.4248	-37.69663	44.65	-20.1	1.1	-10.4	7	0	8	160	19	129
H6	0.9679	-0.62487	47.06	2.3	-0.1	2.2	-1	0	-2	57	27	-215
O6	9.0950	-75.79711	123.20	14.2	2.2	7.0	-6	0	6	-135	36	1492
H(O6)	0.4179	-0.36361	22.75	-2.0	0.0	-1.4	1	0	1	110	-2	136
C7	6.0341	-38.07446	81.24	-0.3	-0.7	5.3	1	0	1	28	55	98
H7	0.9427	-0.60269	46.35	-4.2	0.0	5.0	4	0	-5	298	45	-330
C8	6.0256	-38.04674	83.45	-3.5	0.6	4.3	-2	0	-3	-270	32	-247
H8	0.9561	-0.60788	47.77	-0.5	0.1	9.0	0	0	-9	-26	-32	-620
C9	5.7582	-37.89208	48.51	1.0	1.4	4.5	-2	1	-1	40	123	16
H9	0.9680	-0.62621	46.14	-0.5	0.0	8.7	0	0	-8	-13	88	-601
C10	5.9271	-37.99767	58.45	-2.4	0.8	1.2	1	0	1	145	-46	173
H10e	0.9921	-0.62955	46.18	-1.3	0.0	7.7	0	0	-7	-26	-18	-422
H10a	0.9624	-0.61411	46.91	-1.0	0.0	5.5	0	0	-5	-64	39	-421
C11	6.0189	-38.10463	69.44	-3.5	1.0	7.9	0	0	-5	-84	11	-210
C12	6.0410	-38.26435	59.32	1.8	0.6	6.0	1	0	-3	219	39	-98
C13	5.9579	-38.12286	41.22	1.4	0.9	3.7	0	0	0	138	43	34
C14	5.9474	-38.05309	49.36	-6.2	0.5	4.3	0	0	0	5	-6	151
H14	1.0234	-0.66304	42.09	-2.1	-0.1	5.1	0	0	-5	-163	30	-354
C15	5.9255	-38.02305	55.81	1.6	0.7	1.7	0	1	0	124	31	-57
H15e	0.9618	-0.61499	45.29	0.7	0.0	-6.2	0	0	5	186	-7	327
H15a	1.0037	-0.63259	48.62	-0.8	0.0	3.8	0	0	-4	96	-13	-221
C16	5.7293	-37.90195	53.91	-0.7	1.1	3.9	0	0	-1	28	62	-43
H16e	0.9577	-0.61782	45.76	-0.2	0.0	6.7	0	0	-6	-16	59	-409
H16a	0.9477	-0.61759	42.03	0.4	0.0	-3.3	0	0	2	171	-3	127
N17	7.9547	-55.22483	58.77	-2.6	1.8	1.0	-1	0	1	-13	19	-29
H17	0.5667	-0.45199	27.32	0.3	0.0	4.7	0	0	-3	6	-48	-209
C17	5.6748	-37.86515	62.97	-5.8	1.4	0.0	3	0	1	206	-86	146
Ha+(C17)	0.9414	-0.60546	45.47	0.4	0.0	6.3	0	0	-6	33	-9	-315
Ha-(C17)	0.9393	-0.60487	45.30	0.4	0.0	5.9	0	0	-5	11	65	-369
Hc(C17)	0.9408	-0.60787	43.62	0.2	0.0	-1.6	0	0	1	-19	56	6

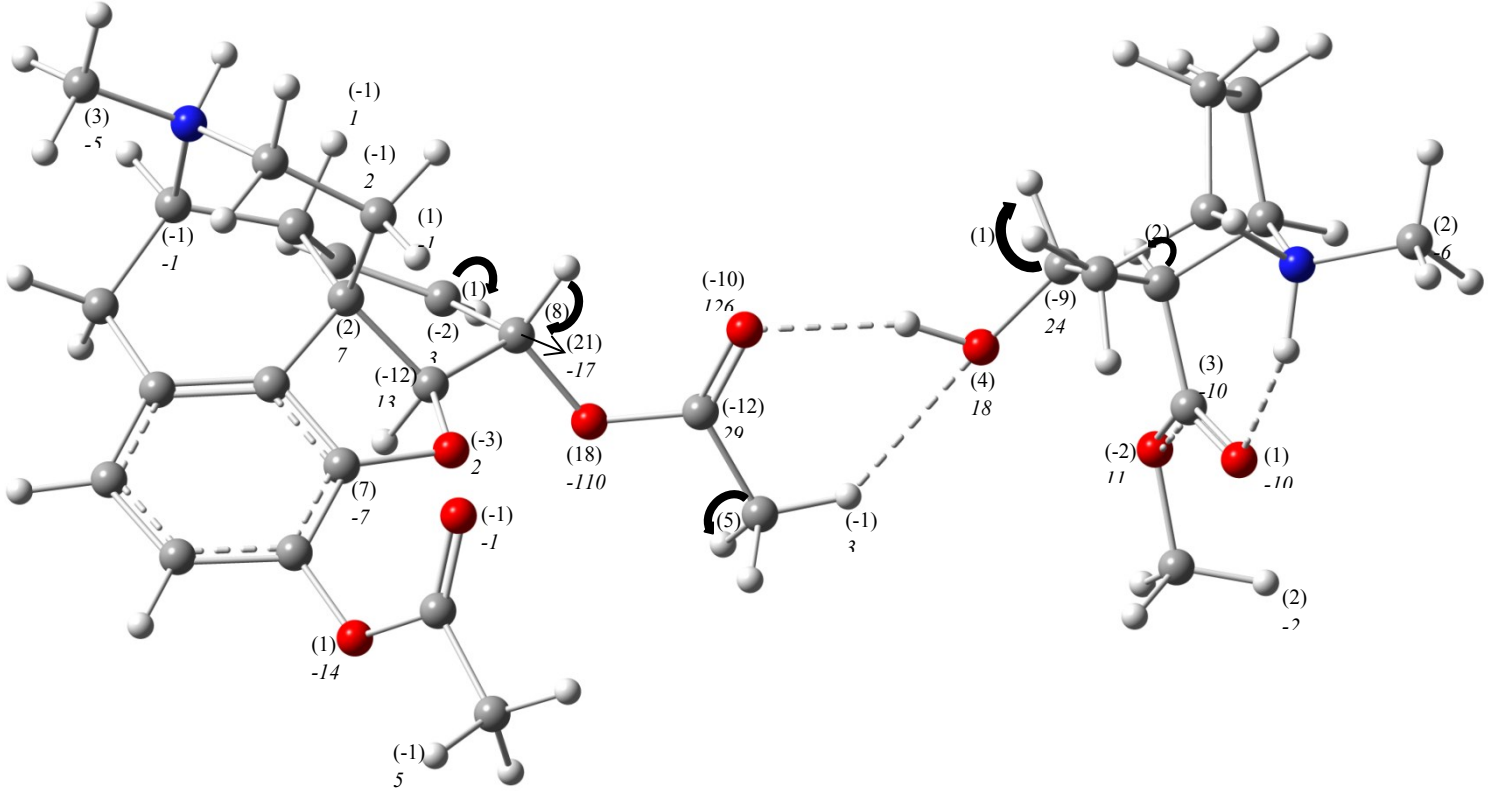
Supplementary Table 2.11a Integrated properties of ecgonine methyl ester in ME5.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b{}^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b{}^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b{}^{CP}v(\Omega)\cdot10^3$
C1	5.7222	-37.91148	46.95	2.3	0.7	3.5	0	-1	1	-45	-48	83
H1	0.9635	-0.62331	45.76	1.6	0.0	-1.2	-2	0	1	-124	8	93
C2	5.9508	-38.08010	48.59	-4.9	-0.3	7.9	-2	0	-1	-253	-10	86
H2	0.9582	-0.61982	44.48	-3.8	-0.1	7.1	1	0	-6	-324	-8	-399
C1'	4.3833	-37.02928	33.78	4.4	-12.9	7.8	-2	0	3	-32	-3	-25
O1'	9.2352	-76.00284	121.54	56.2	0.5	-57.9	-1	0	28	2826	-143	-4836
O2'	9.0967	-75.98065	99.72	-29.1	2.5	17.7	6	0	-8	-194	-41	-420
C3'	5.5361	-37.75872	62.67	7.9	1.6	2.8	-5	0	-1	-90	-30	4
Ht(C3')	0.9347	-0.60678	44.93	-3.1	0.1	12.8	2	0	-11	151	-9	-632
Hg+(C3')	0.9552	-0.61352	46.11	-0.3	0.0	-5.7	1	0	5	119	20	356
Hg-(C3')	0.9530	-0.61215	46.24	-0.3	0.0	-8.9	1	0	8	235	36	505
C3	5.4373	-37.69770	41.82	0.0	1.4	1.6	-1	0	0	12	78	46
H3	0.9953	-0.64443	45.02	-2.6	0.1	8.0	1	0	-7	50	-11	-432
O3	9.1131	-75.81967	119.55	-0.8	3.5	2.3	0	0	5	10	-109	520
H(O3)	0.3964	-0.35324	20.69	1.6	-0.1	5.0	-1	0	-3	-100	18	-213
C4	5.9259	-38.05011	54.75	-3.2	-0.9	3.5	0	0	-1	-7	116	-86
H4a	0.9769	-0.62198	46.04	-1.0	-0.1	-8.4	1	0	7	166	-52	1052
H4e	0.9655	-0.61539	46.89	0.8	-0.1	1.7	0	0	-1	27	-16	-71
C5	5.7229	-37.91319	48.08	-8.0	0.6	7.7	4	-1	-2	272	-95	73
H5	0.9643	-0.62327	46.02	-0.1	0.0	0.2	0	0	0	11	30	186
C6	5.9363	-38.01613	58.07	-2.2	0.8	3.0	0	0	0	-48	0	-11
H6a	0.9754	-0.62118	46.40	0.9	-0.2	3.1	-1	0	-3	-130	-1	-193
H6e	0.9869	-0.62819	47.22	-0.1	0.0	2.8	0	0	-3	-125	-15	-185
C7	5.9354	-38.01482	57.97	-5.2	1.4	4.0	-1	0	0	-157	8	1
H7e	0.9822	-0.62627	46.97	-1.0	0.0	4.9	0	0	-4	-83	3	-378
H7a	0.9778	-0.62250	46.20	0.7	-0.1	3.0	-1	0	-3	-131	-6	-293
N8	8.0225	-55.34688	58.79	18.9	1.6	9.2	-9	1	-3	-238	142	-771
H8	0.4933	-0.40735	16.38	-16.3	-0.6	-2.0	12	0	-2	2027	19	-2754
C8	5.6585	-37.85581	63.49	-11.6	0.3	9.3	1	-1	-4	-67	-103	-336
Ha-(C8)	0.9405	-0.60581	45.82	-2.2	-0.4	4.8	0	0	-4	-92	12	92
Ha+(C8)	0.9490	-0.60851	46.29	0.6	-0.2	-5.3	-1	0	5	-167	11	497
Hc(C8)	0.9547	-0.61449	43.92	2.5	-0.1	-1.7	-3	0	1	-325	-18	-19

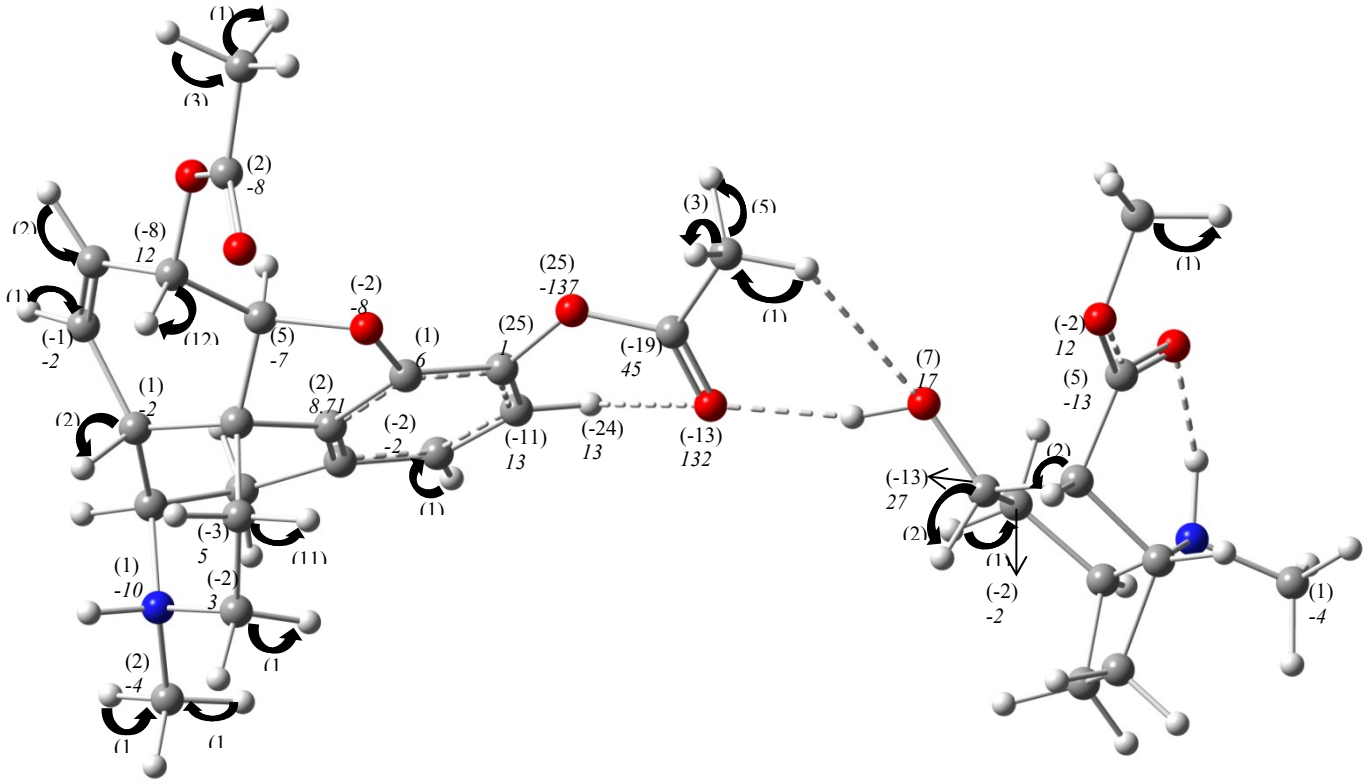
Supplementary Table 2.11b Integrated properties of morphine in ME5.

Atom	$N(\Omega)$	$E(\Omega)$	$v(\Omega)$	$\Delta_{def}E(\Omega)$	$-\Delta_{BSSE}E(\Omega)$	$\Delta_b^{CP}E(\Omega)$	$\Delta_{def}N(\Omega)10^3$	$-\Delta_{BSSE}N(\Omega)\cdot10^3$	$\Delta_b^{CP}N(\Omega)\cdot10^3$	$\Delta_{def}V(\Omega)\cdot10^3$	$-\Delta_{BSSE}v(\Omega)\cdot10^3$	$\Delta_b^{CP}v(\Omega)\cdot10^3$
C1	5.9898	-38.03267	83.59	-7.0	0.4	5.4	0	0	-4	-66	37	-335
H1	0.9666	-0.61339	48.21	-0.7	0.0	10.2	0	0	-10	6	-15	-685
C2	5.9761	-38.03688	82.53	-6.6	0.1	5.2	0	0	-3	-4	18	-168
H2	0.9353	-0.60101	45.73	0.2	0.0	8.1	0	0	-8	3	-49	-480
C3	5.4133	-37.72037	59.20	-4.9	-0.1	1.5	0	0	1	1	-9	18
O3	9.1298	-75.88003	121.85	-6.2	2.4	9.0	-1	0	-3	36	-40	-128
H(O3)	0.3876	-0.34809	20.27	-0.2	0.3	-9.3	-1	0	6	-54	13	348
C4	5.5810	-37.90040	60.75	-18.3	1.1	-7.7	11	0	8	274	13	170
O	9.0190	-75.77097	106.22	16.8	1.9	-5.1	-6	0	11	149	-53	528
C5	5.5562	-37.87514	41.35	11.8	-0.9	4.9	-9	-1	1	-247	-235	-52
H5	0.9925	-0.65116	42.62	-1.2	0.1	2.2	0	0	-1	-7	-63	59
C6	5.4423	-37.70634	45.02	-34.8	-4.8	-15.0	23	-2	13	739	-166	115
H6	0.9743	-0.62733	47.78	5.9	-0.1	-7.8	-4	0	7	-23	29	588
O6	9.1430	-75.81098	122.78	76.0	-3.5	-85.8	-14	1	61	274	-134	831
H(O6)	0.3899	-0.34772	18.63	0.9	0.2	37.1	2	0	-28	209	159	-4237
C7	6.0344	-38.07484	81.56	0.4	-3.8	6.5	-2	-1	5	73	-36	454
H7	0.9522	-0.60700	46.97	-0.4	0.1	-10.2	0	0	9	-34	20	646
C8	6.0215	-38.04525	83.27	-6.6	-1.3	13.3	1	0	-10	-92	21	-597
H8	0.9564	-0.60820	47.75	-1.8	0.1	9.4	1	0	-10	-29	-13	-658
C9	5.7578	-37.89172	48.42	0.4	0.7	6.7	-1	0	-1	65	54	-30
H9	0.9692	-0.62663	46.23	0.3	0.0	6.8	0	0	-6	-13	15	-442
C10	5.9252	-37.99817	58.31	-5.6	0.8	3.2	0	0	-1	20	-2	114
H10e	0.9910	-0.62919	46.09	-1.8	0.0	9.2	1	0	-8	-54	-21	-483
H10a	0.9648	-0.61499	47.09	0.1	0.0	2.2	0	0	-2	-51	-35	-165
C11	6.0201	-38.10654	69.33	-5.3	-0.2	5.8	0	0	-3	-236	57	-206
C12	6.0424	-38.26647	59.10	-1.4	0.9	3.3	-1	0	0	-43	9	-22
C13	5.9584	-38.12093	41.42	2.7	0.3	7.9	0	0	1	179	42	201
C14	5.9475	-38.05277	49.35	-3.7	-0.4	3.6	1	-1	1	130	-85	89
H14	1.0249	-0.66339	42.23	-2.1	0.0	4.2	0	0	-4	-107	-13	-221
C15	5.9258	-38.02283	55.83	1.7	-0.2	2.8	0	0	1	134	-4	-11
H15e	0.9577	-0.61369	44.78	-0.8	0.0	-1.4	1	0	1	80	18	-104
H15a	1.0096	-0.63453	49.15	1.1	0.0	-3.1	0	0	3	161	2	229
C16	5.7292	-37.90174	53.84	-1.3	0.9	5.2	0	0	-1	32	-56	10
H16e	0.9574	-0.61785	45.68	-0.7	0.0	7.2	0	0	-7	-26	-32	-406
H16a	0.9415	-0.61479	41.62	0.2	0.0	4.2	0	0	-4	73	-3	-204
N17	7.9544	-55.22392	58.75	-1.0	1.0	2.6	-1	0	1	0	-37	-22
H17	0.5692	-0.45347	27.39	0.5	0.0	0.6	0	0	-1	-19	-5	-136
C17	5.6753	-37.86492	63.05	-6.3	0.9	1.7	3	0	2	188	-11	175
Ha+(C17)	0.9416	-0.60544	45.50	0.7	0.0	6.0	-1	0	-5	-1	-4	-268
Ha-(C17)	0.9384	-0.60450	45.26	0.1	0.0	7.2	0	0	-6	-20	15	-325
Hc(C17)	0.9374	-0.60643	43.47	-0.1	0.0	2.4	0	0	-2	14	-13	-102

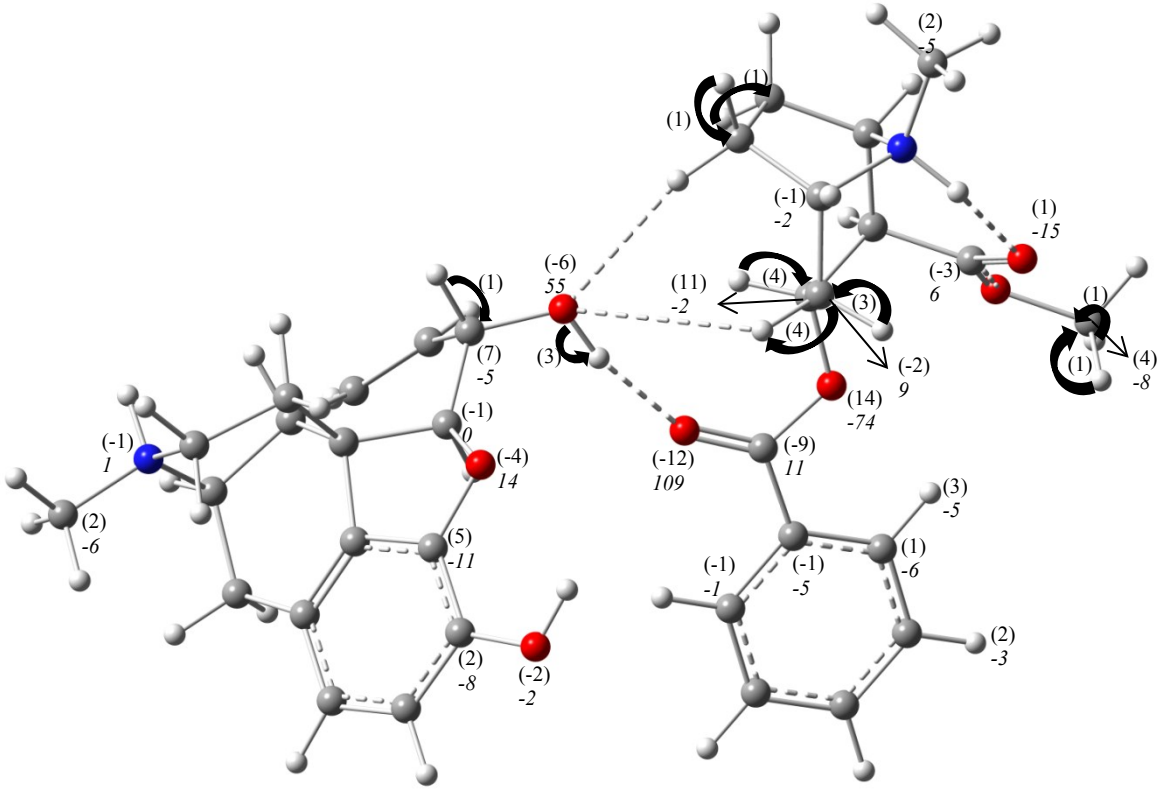
Supplementary Figure 1 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **HE1**.



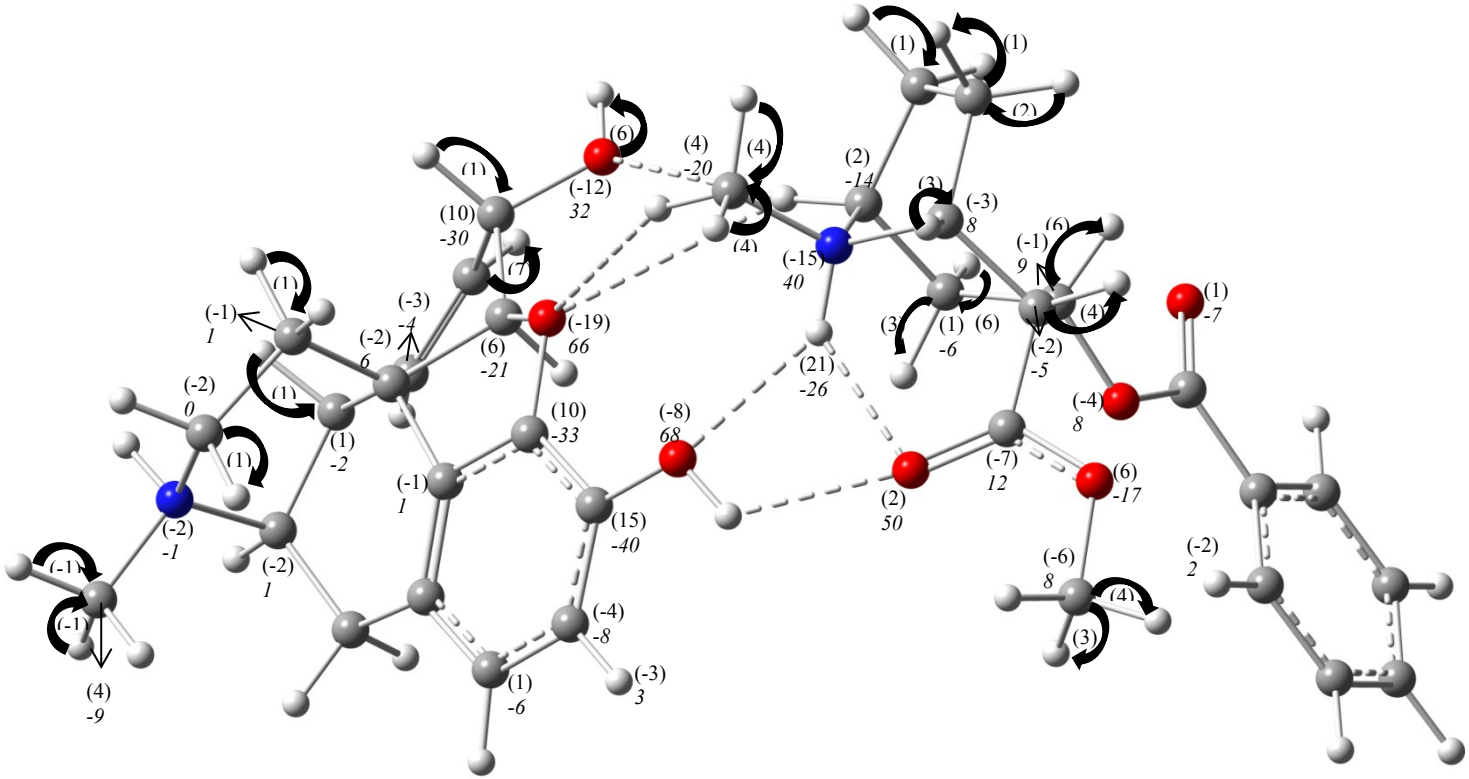
Supplementary Figure 2 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **HE2**.



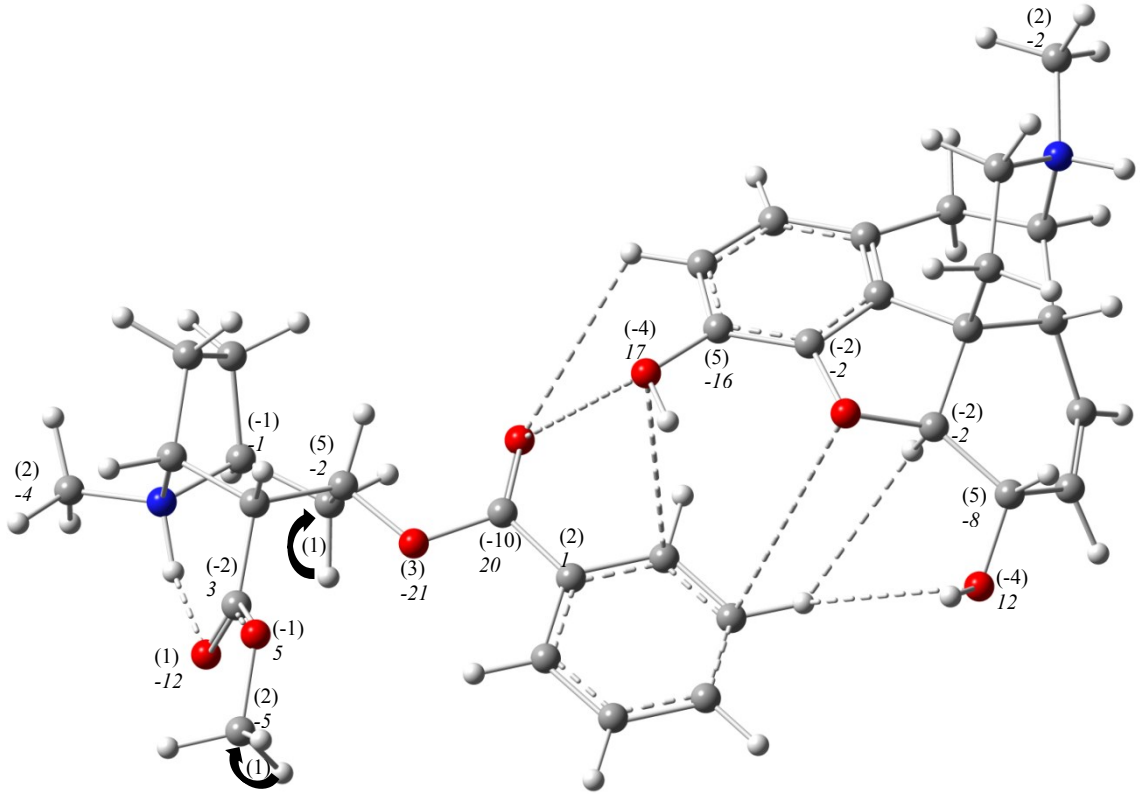
Supplementary Figure 3 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **MC1**.



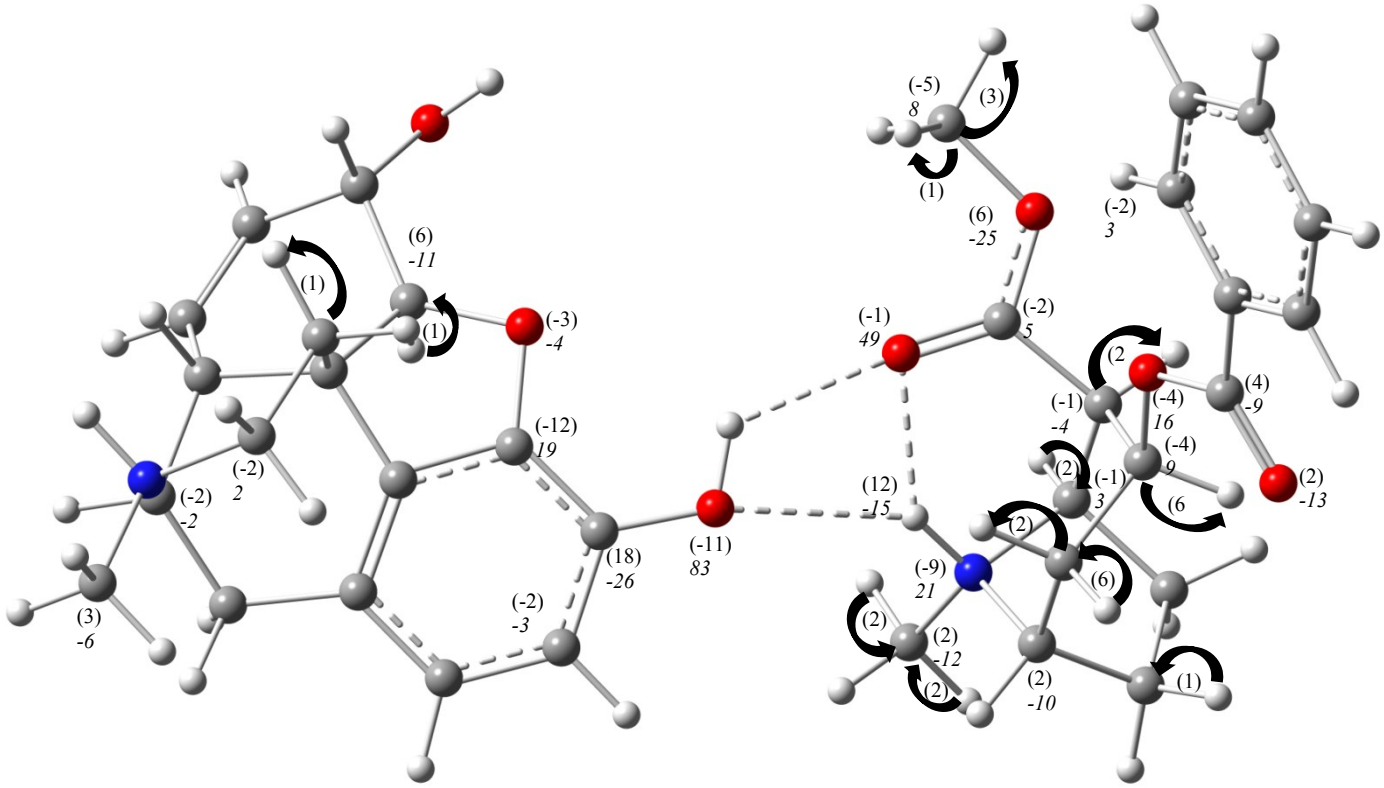
Supplementary Figure 4 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **MC2**.



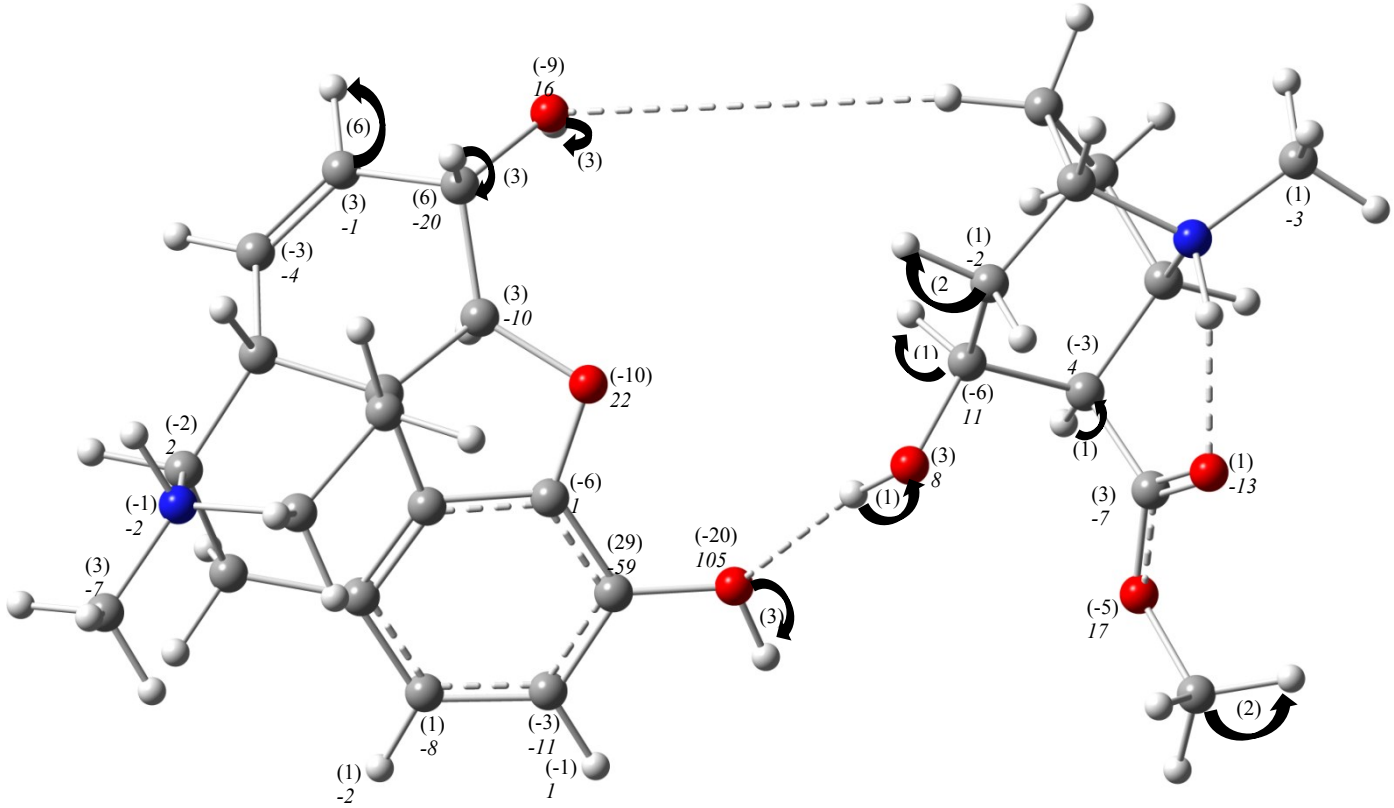
Supplementary Figure 5 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **MC3**.



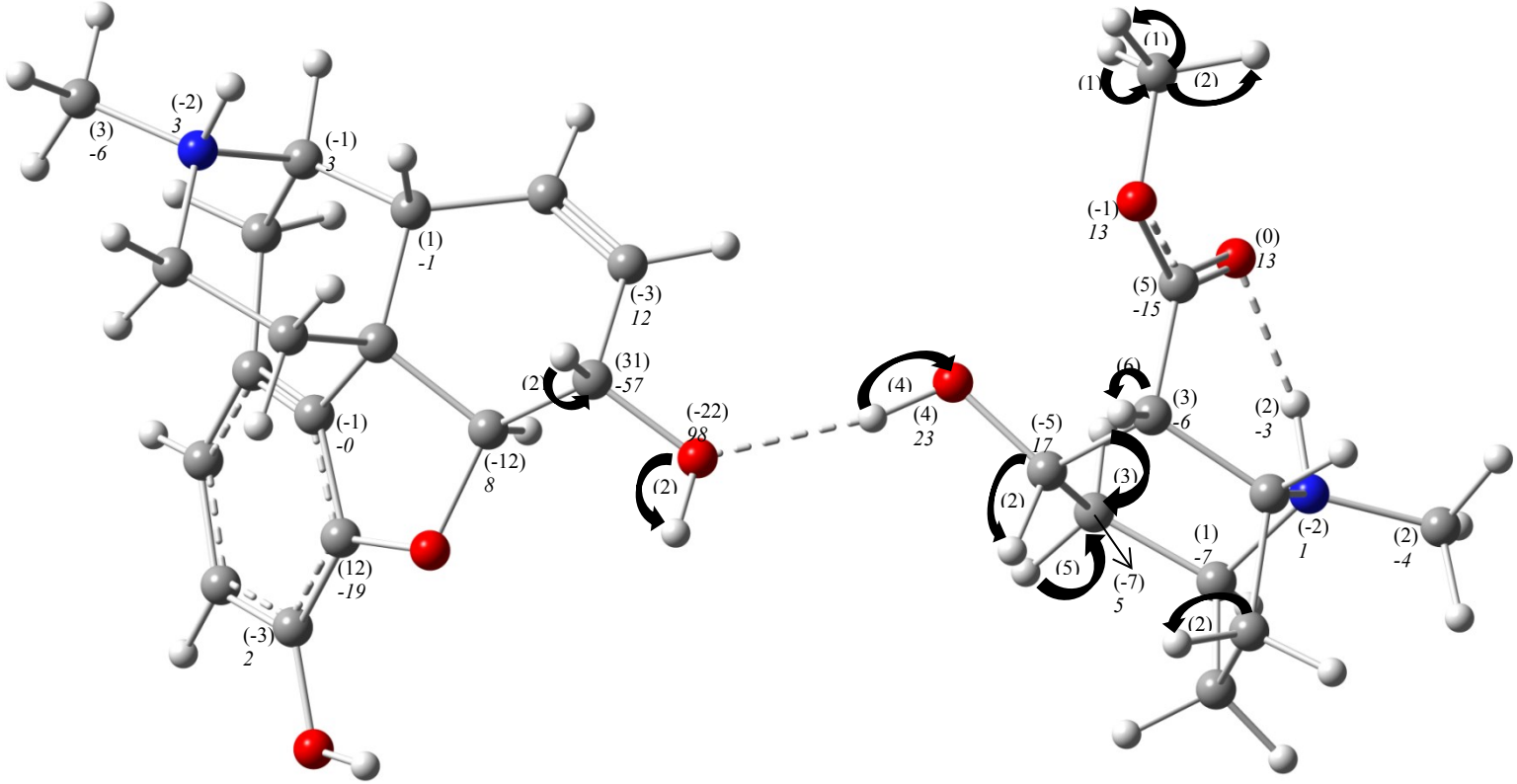
Supplementary Figure 6 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **MC4**.



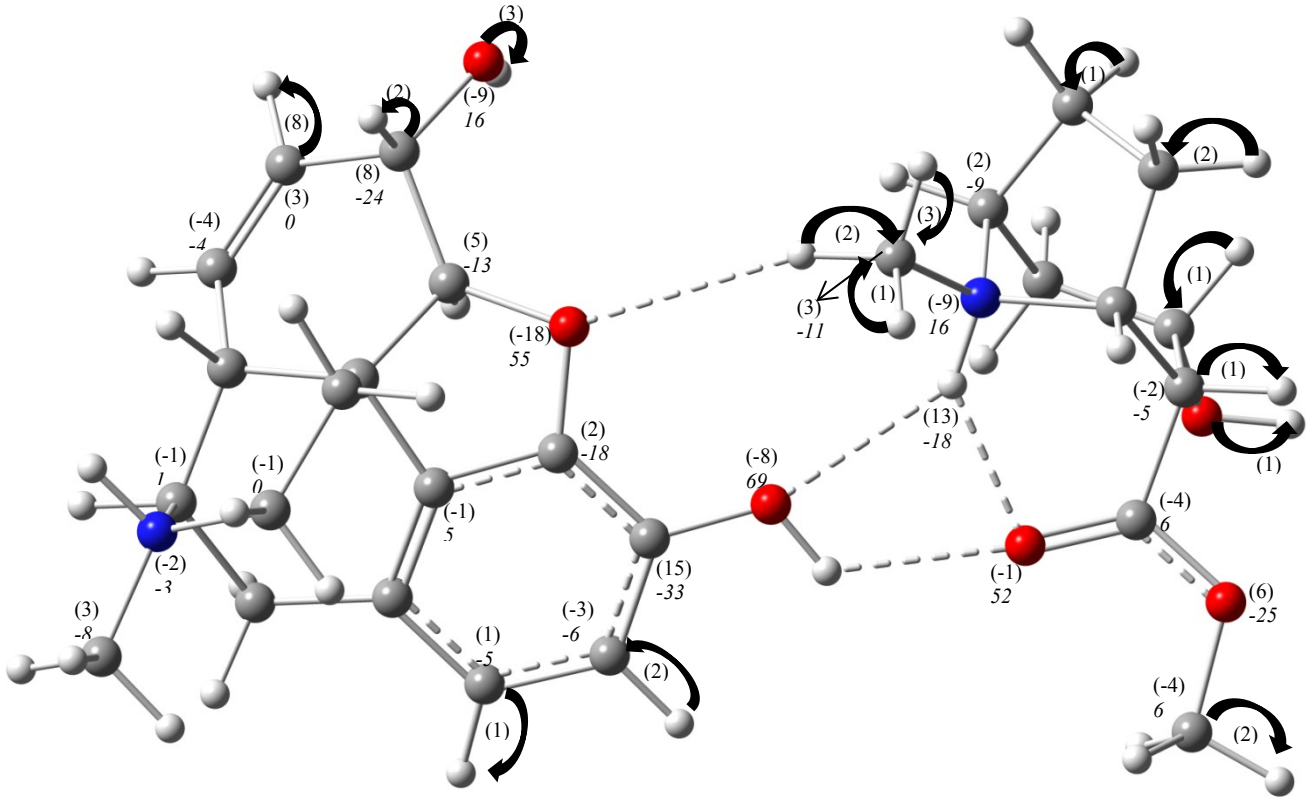
Supplementary Figure 7 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **ME1**.



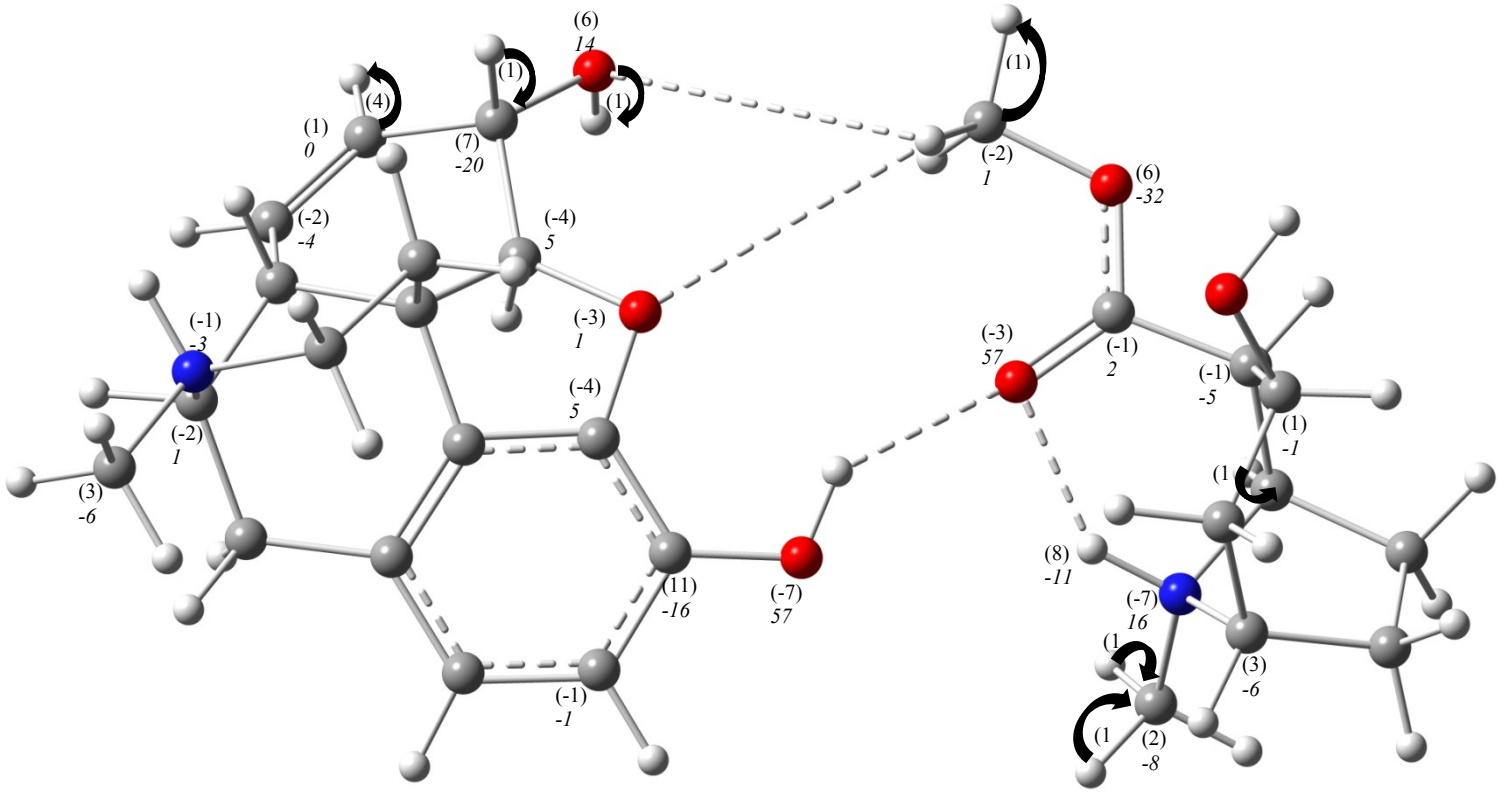
Supplementary Figure 8 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **ME2**.



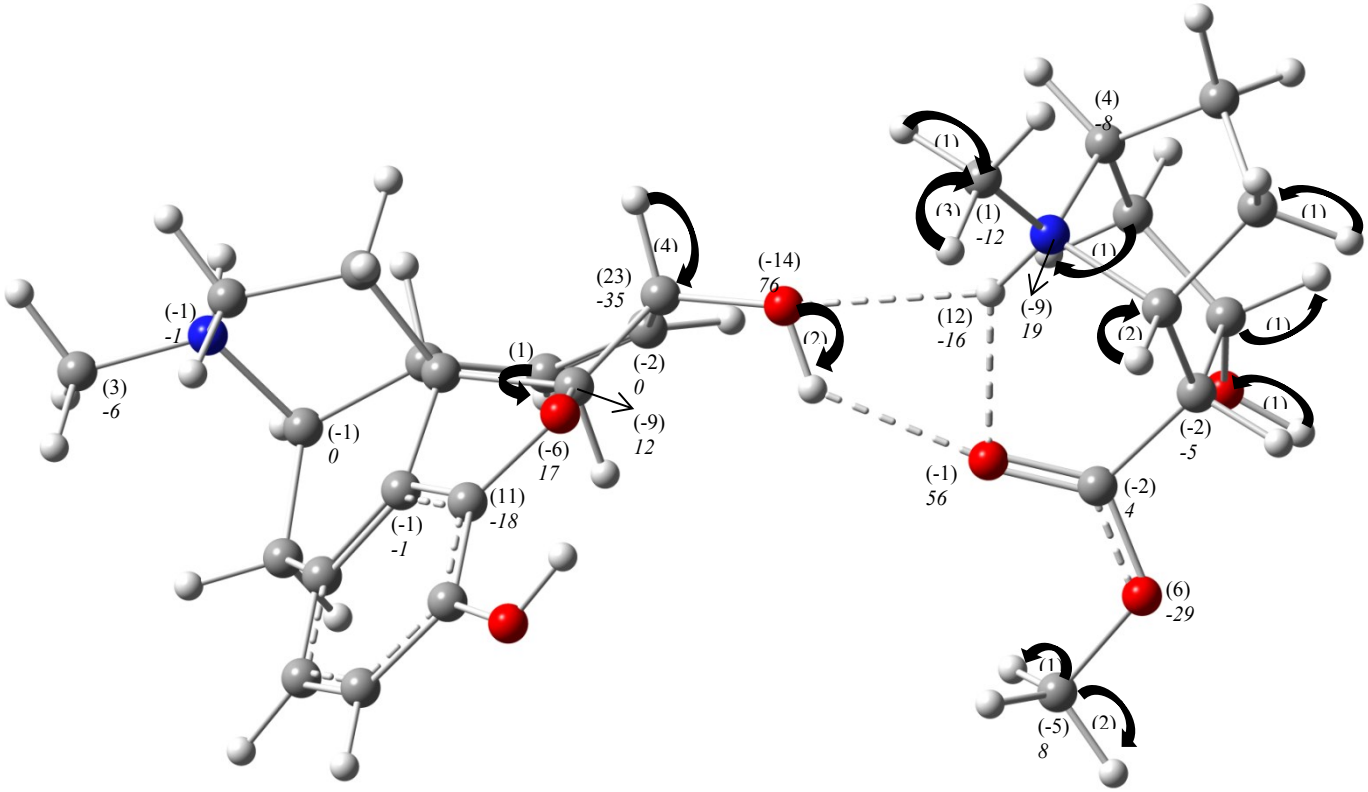
Supplementary Figure 9 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **ME3**.



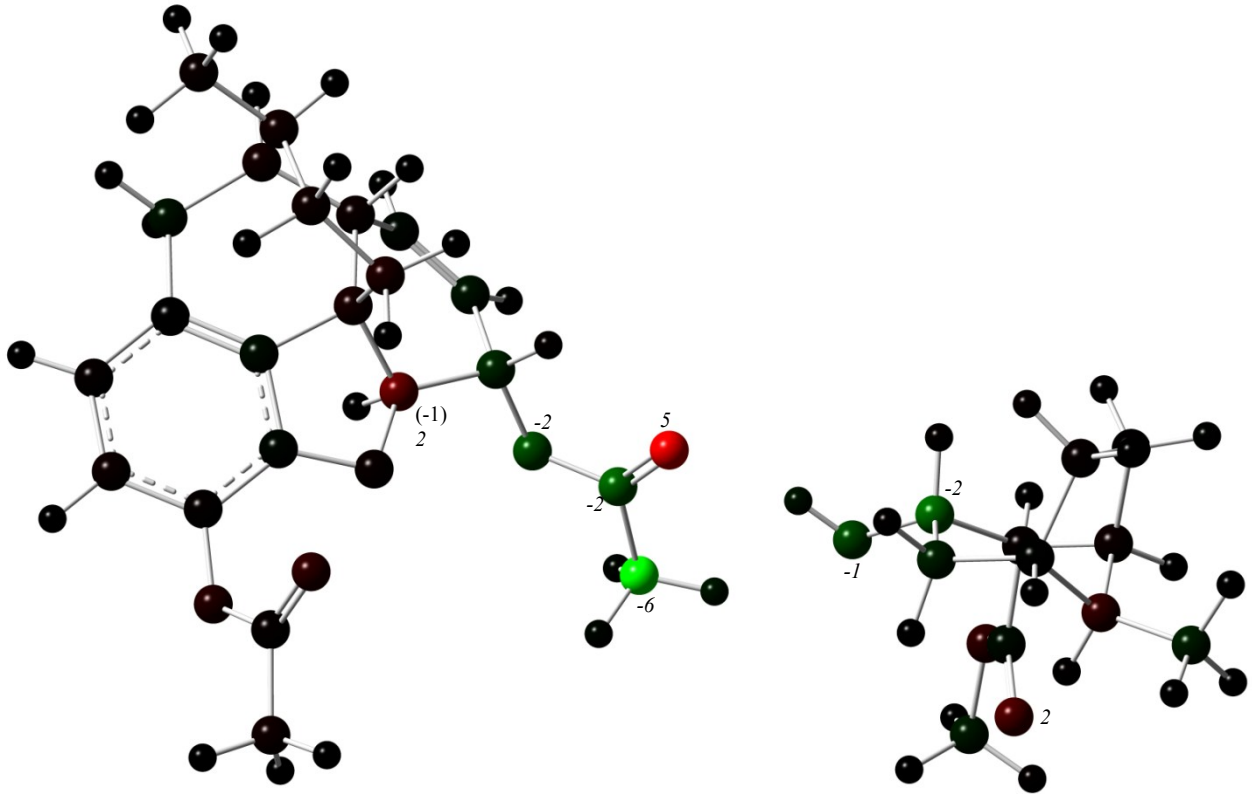
Supplementary Figure 10 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **ME4**.



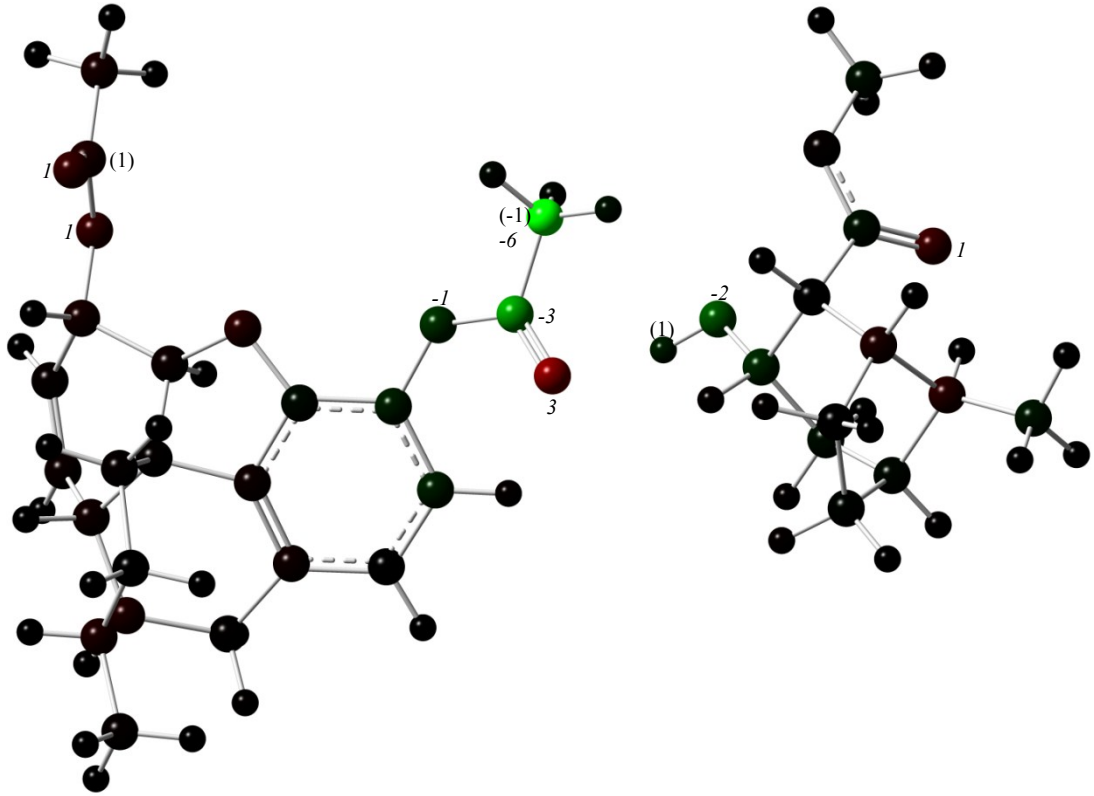
Supplementary Figure 11 Principal $\Delta_{def}N(\Omega)$ (in au multiplied by 10^3) and $\Delta_{def}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **ME5**.



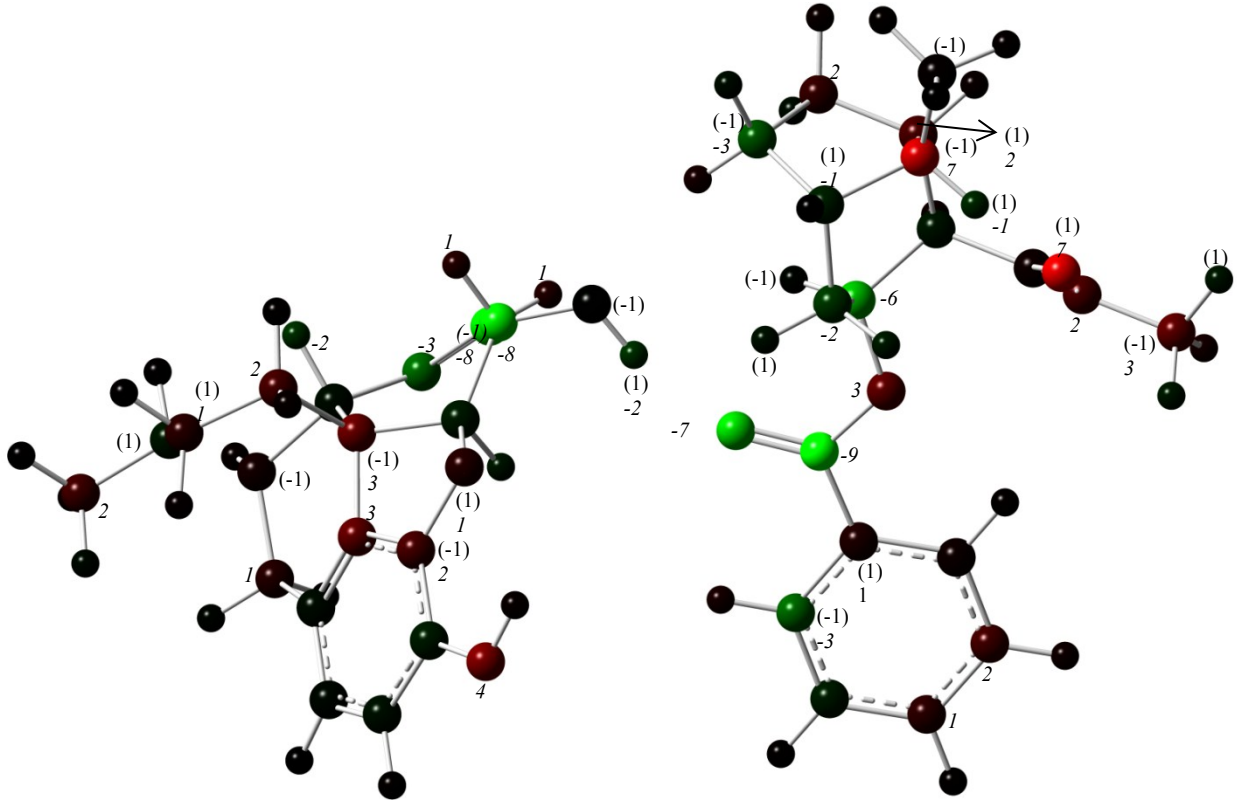
Supplementary Figure 12 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **HE1**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



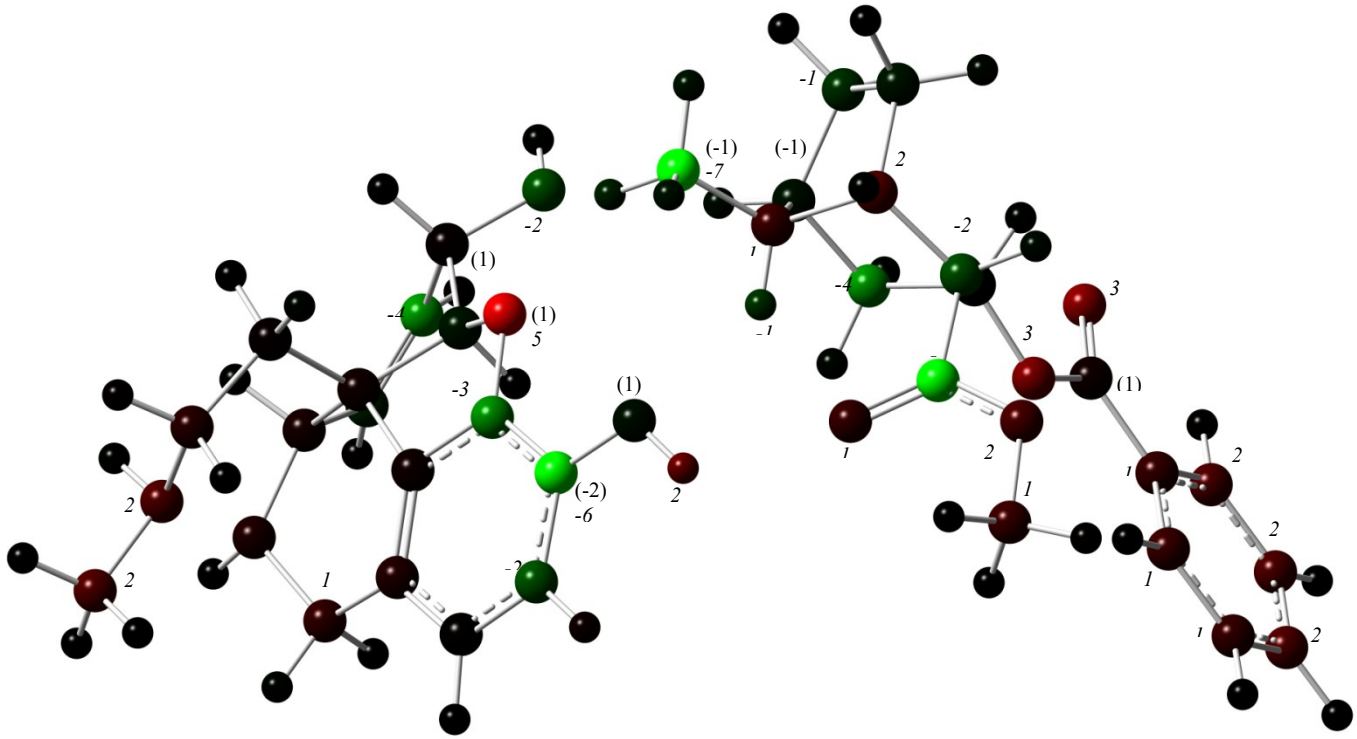
Supplementary Figure 13 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **HE2**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



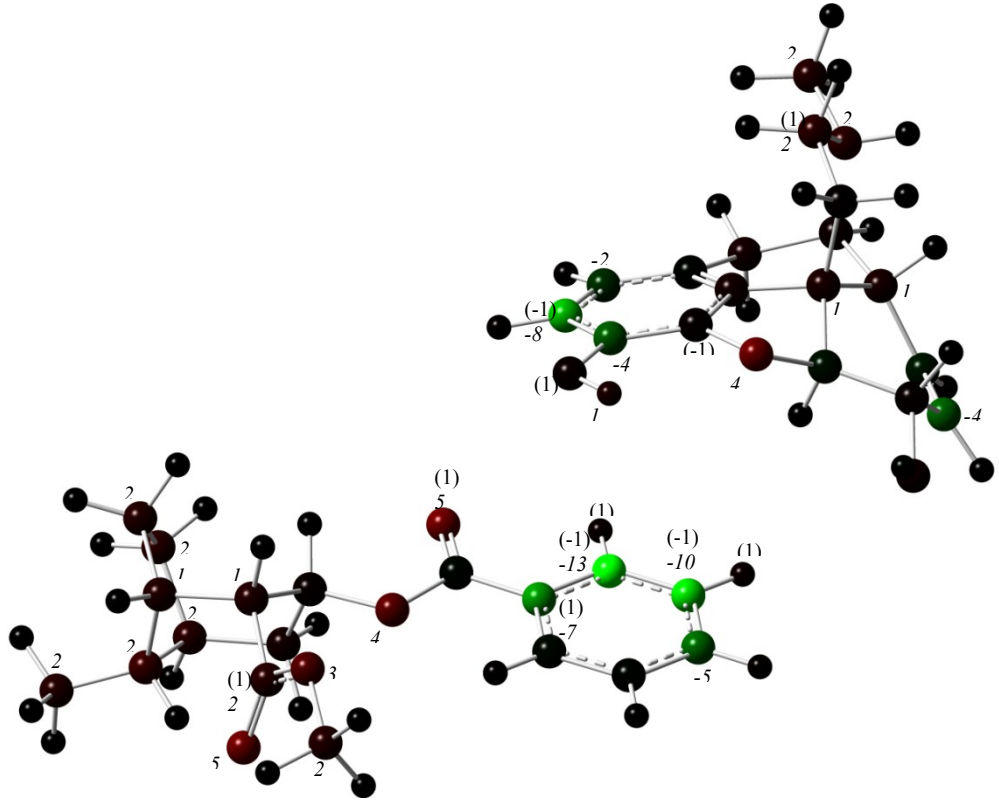
Supplementary Figure 14 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **MC1**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



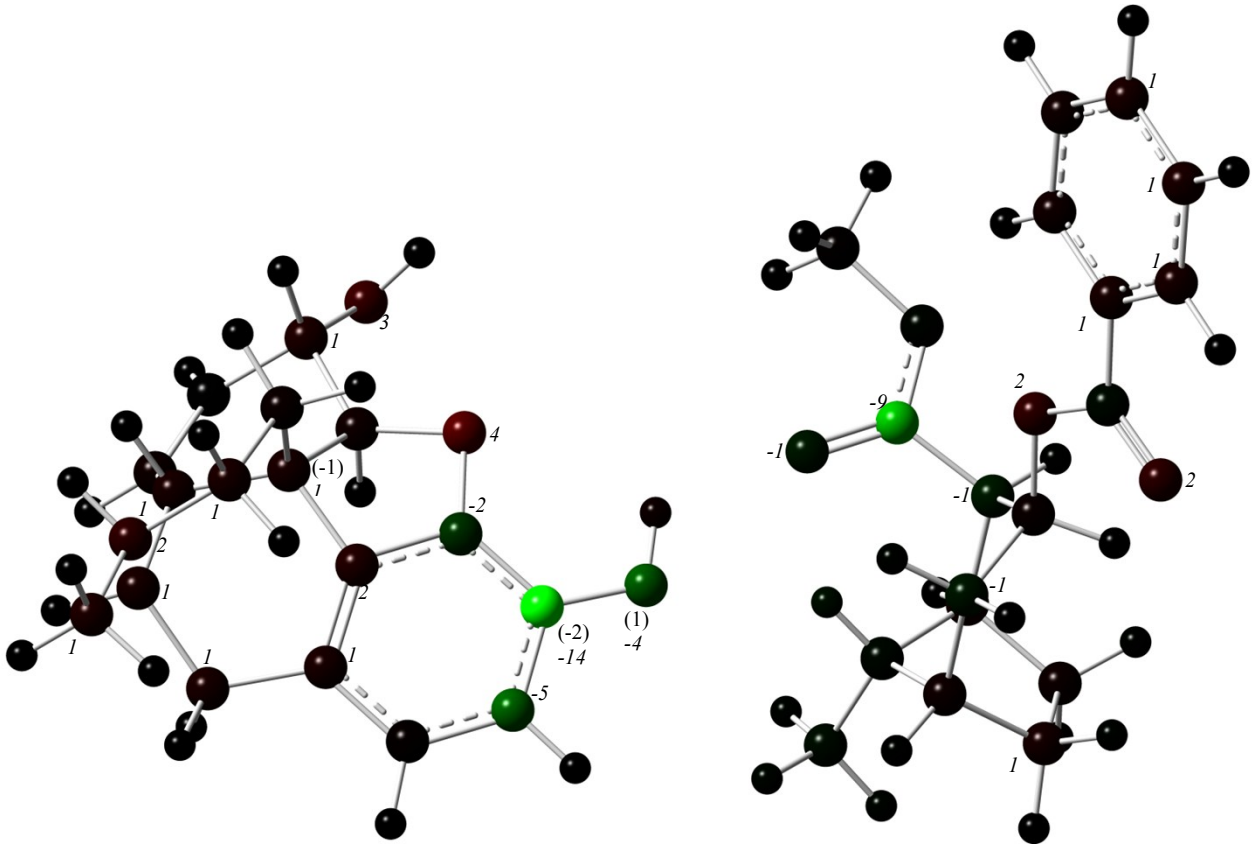
Supplementary Figure 15 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **MC2**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



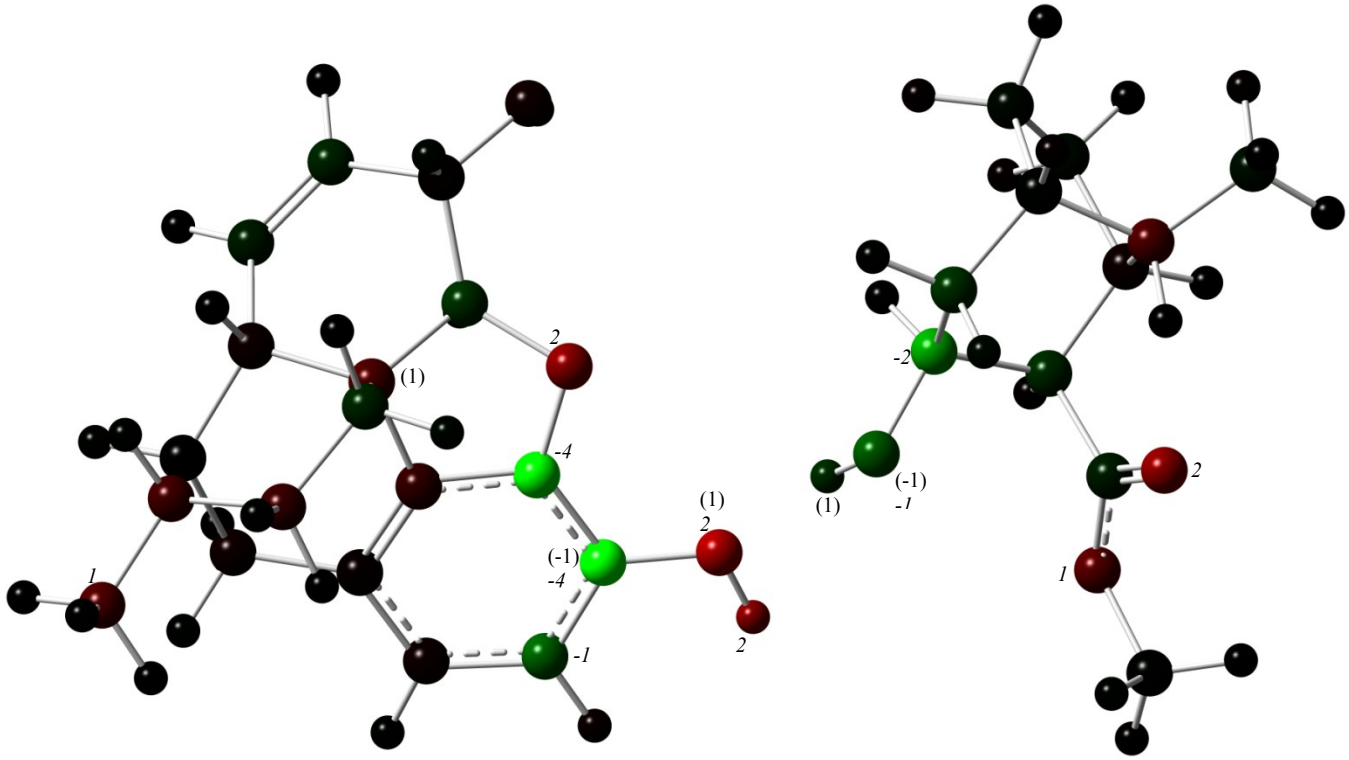
Supplementary Figure 16 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **MC3**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



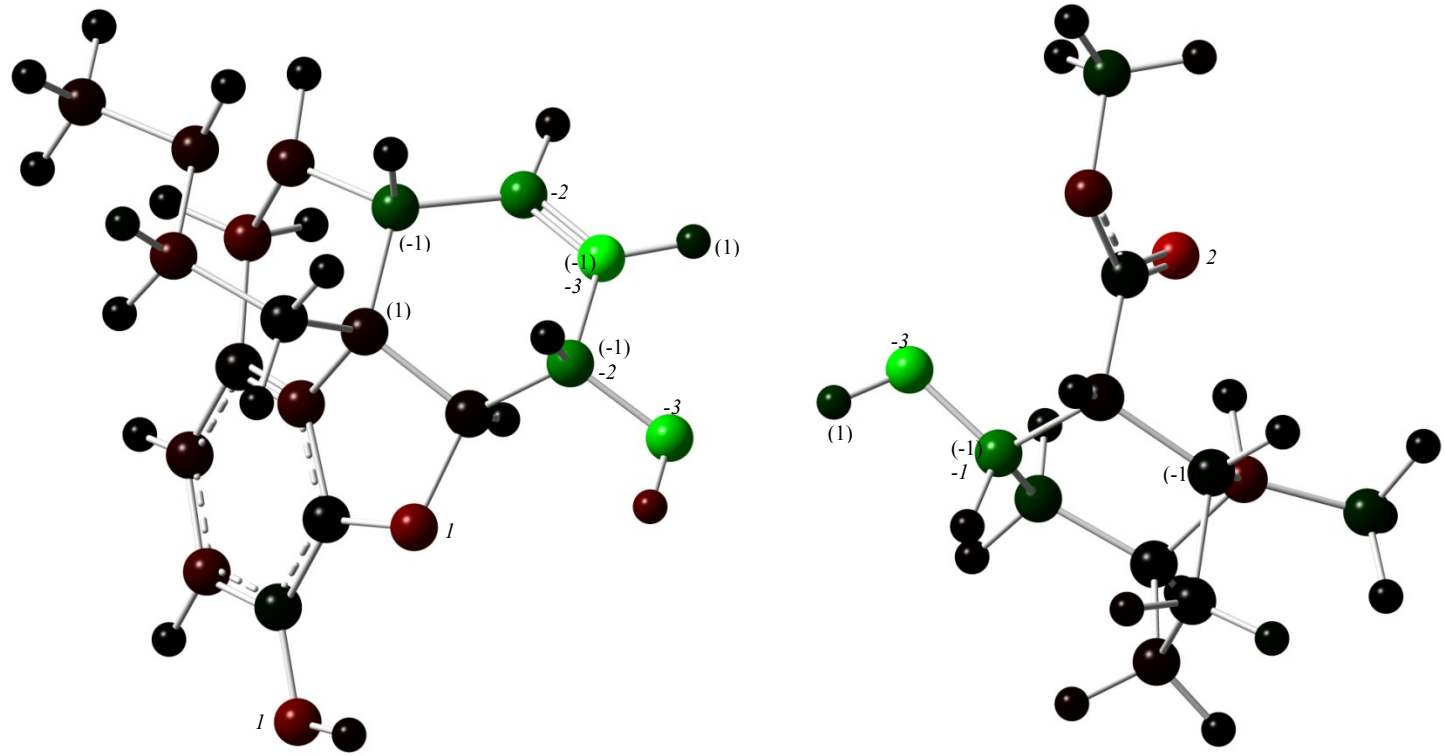
Supplementary Figure 17 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **MC4**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



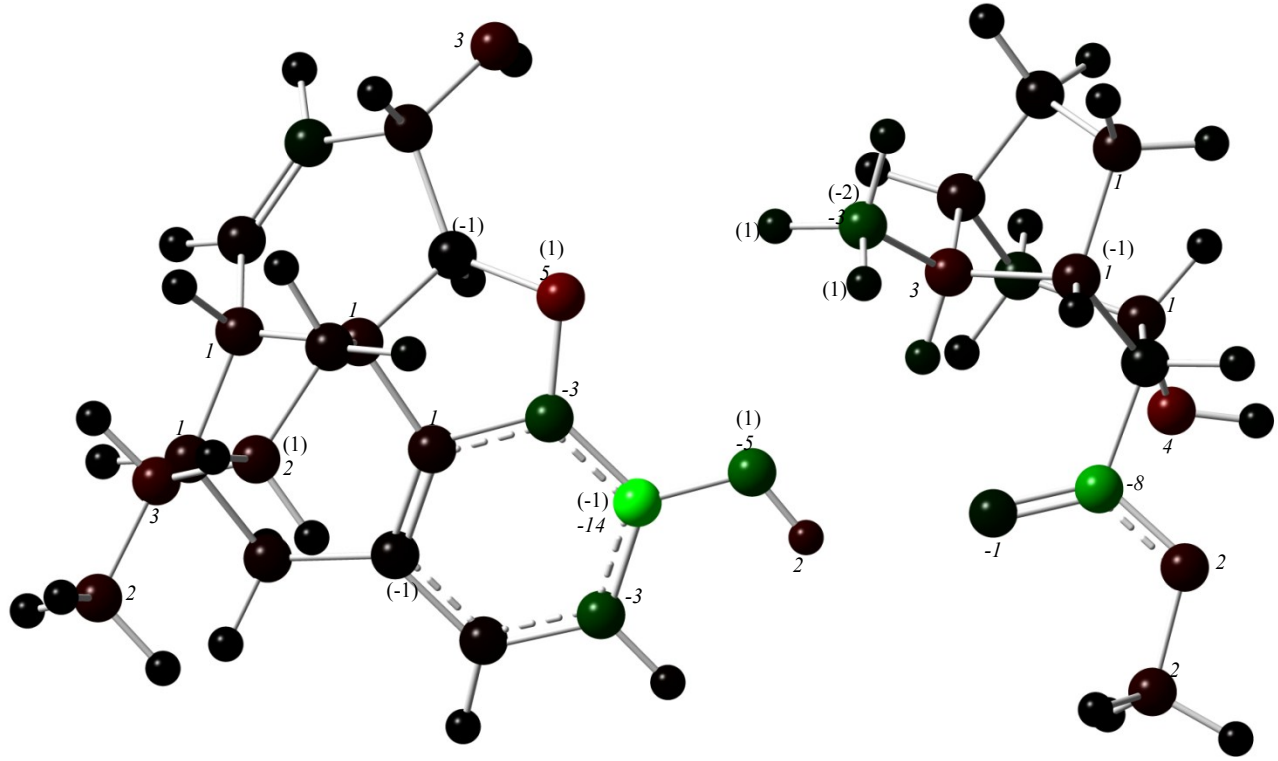
Supplementary Figure 18 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **ME1**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



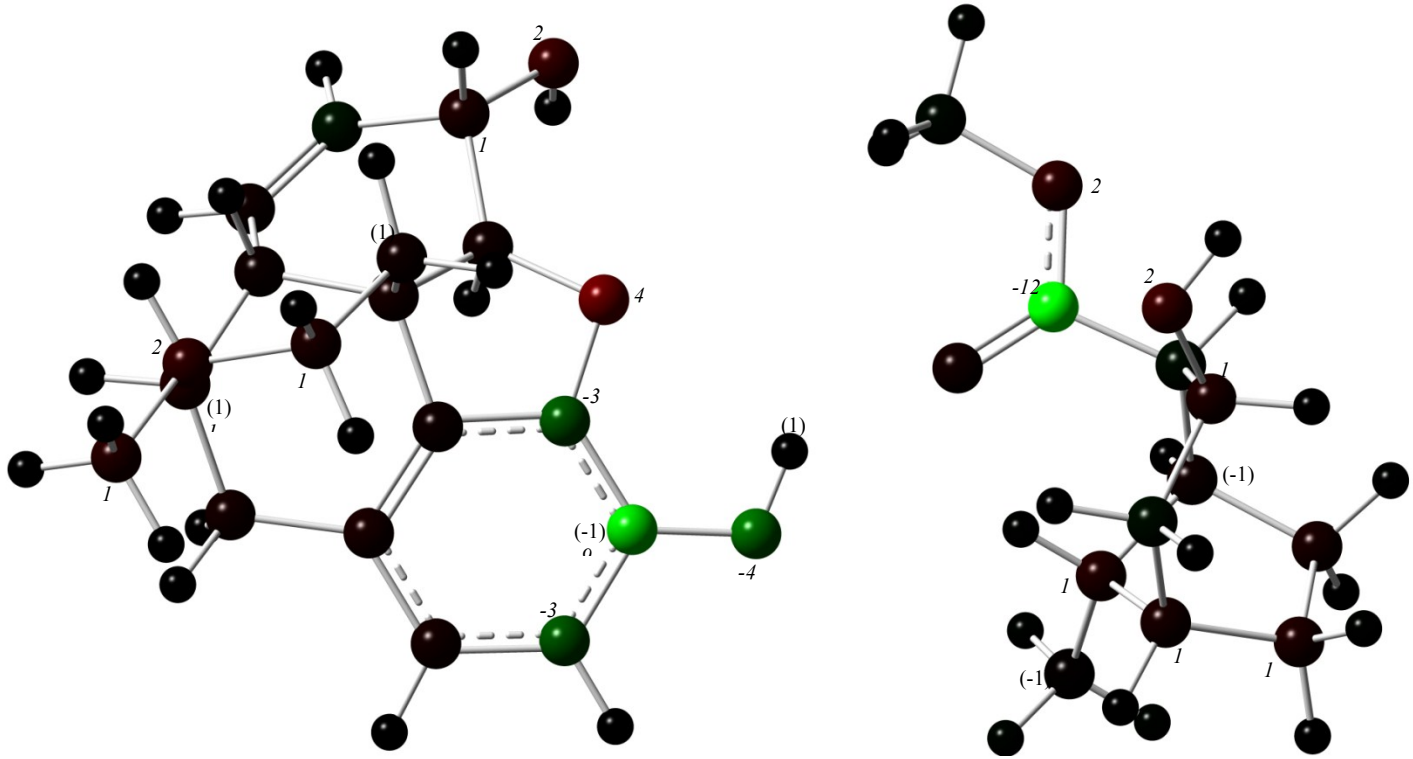
Supplementary Figure 19 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **ME2**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



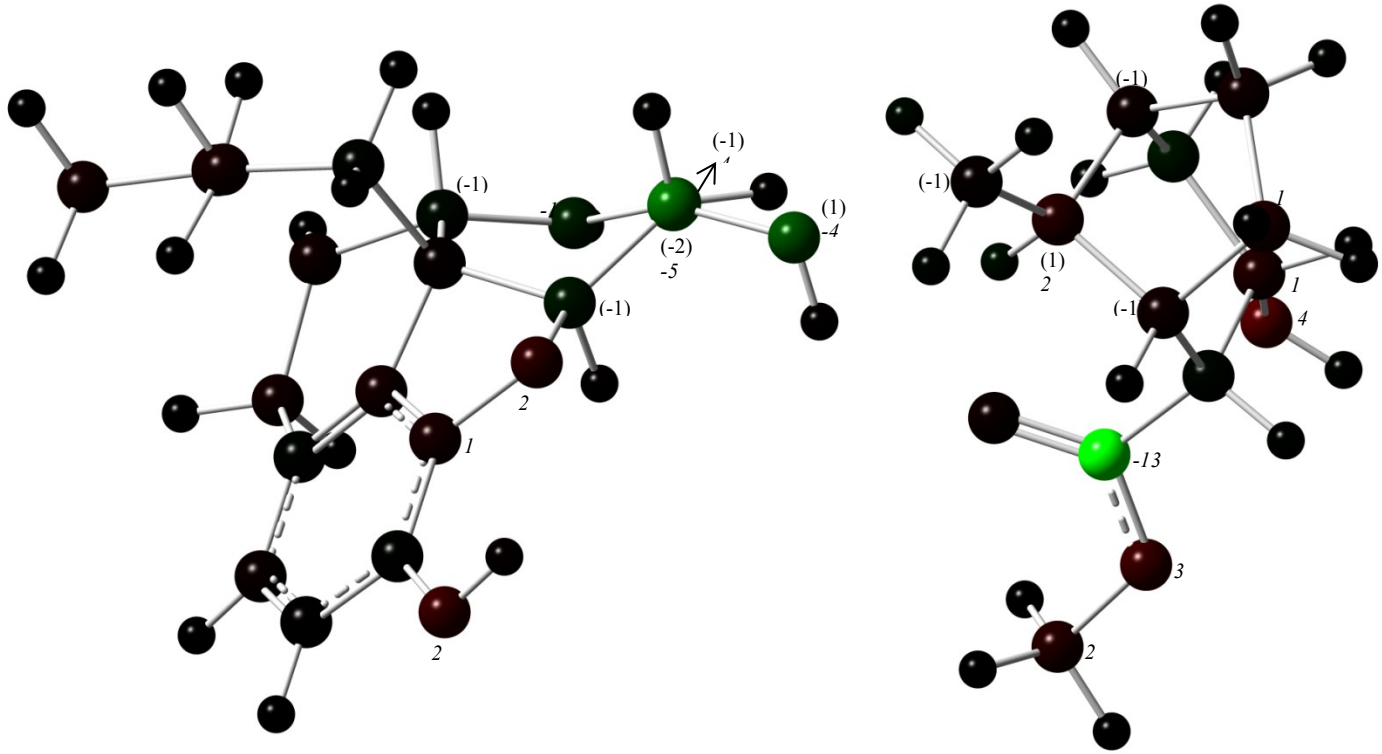
Supplementary Figure 20 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **ME3**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



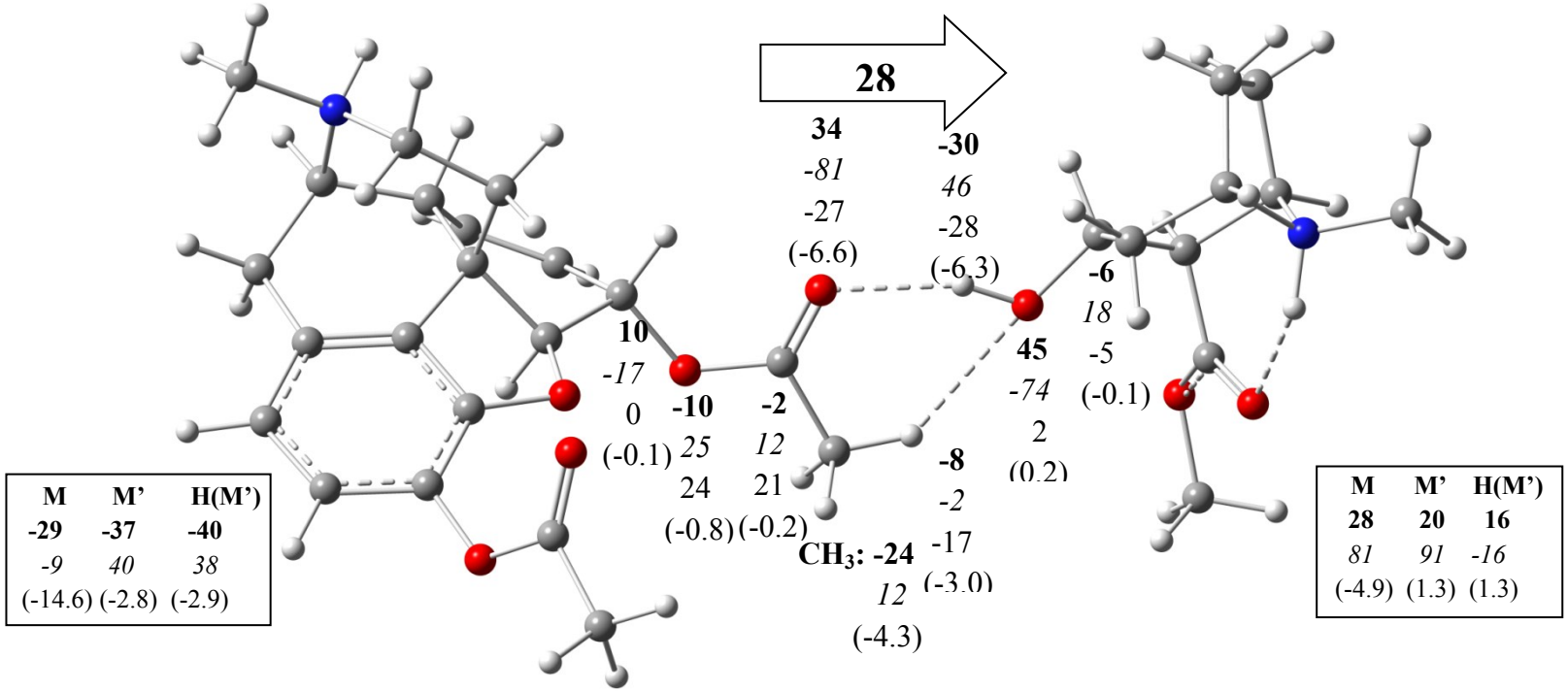
Supplementary Figure 21 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **ME4**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



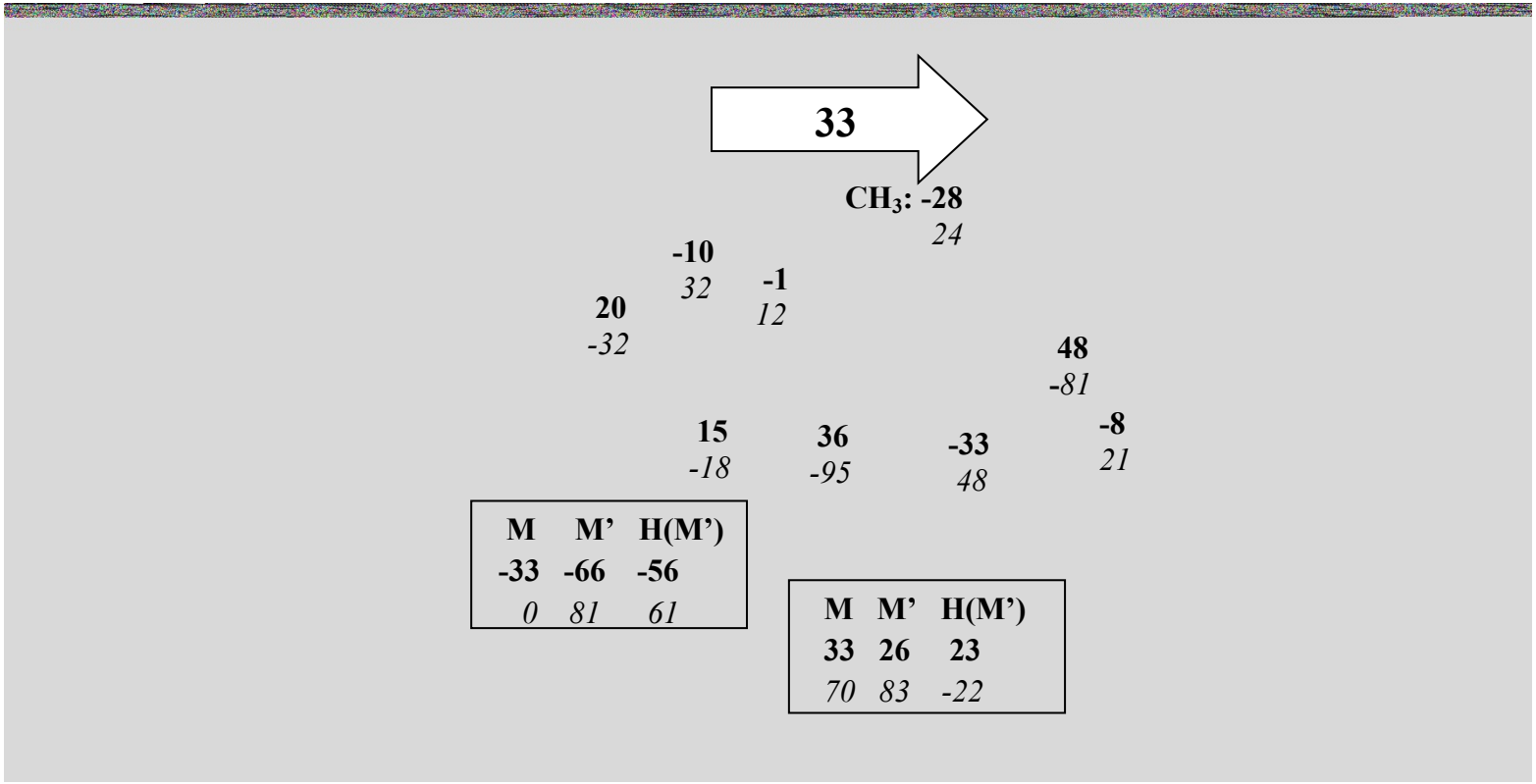
Supplementary Figure 22 Principal $-\Delta_{BSSE}N(\Omega)$ (in au and multiplied by 10^3) and $-\Delta_{BSSE}E(\Omega)$ (in italics and expressed in kJ mol^{-1}) values for **ME5**. Reddish colour atoms indicate atoms where $\Delta_c^{CP}E(\Omega) > \Delta_c E(\Omega)$, while greenish ones are the atoms extra-stabilized according to CP-uncorrected atomic energies, that is: $\Delta_c^{CP}E(\Omega) < \Delta_c E(\Omega)$.



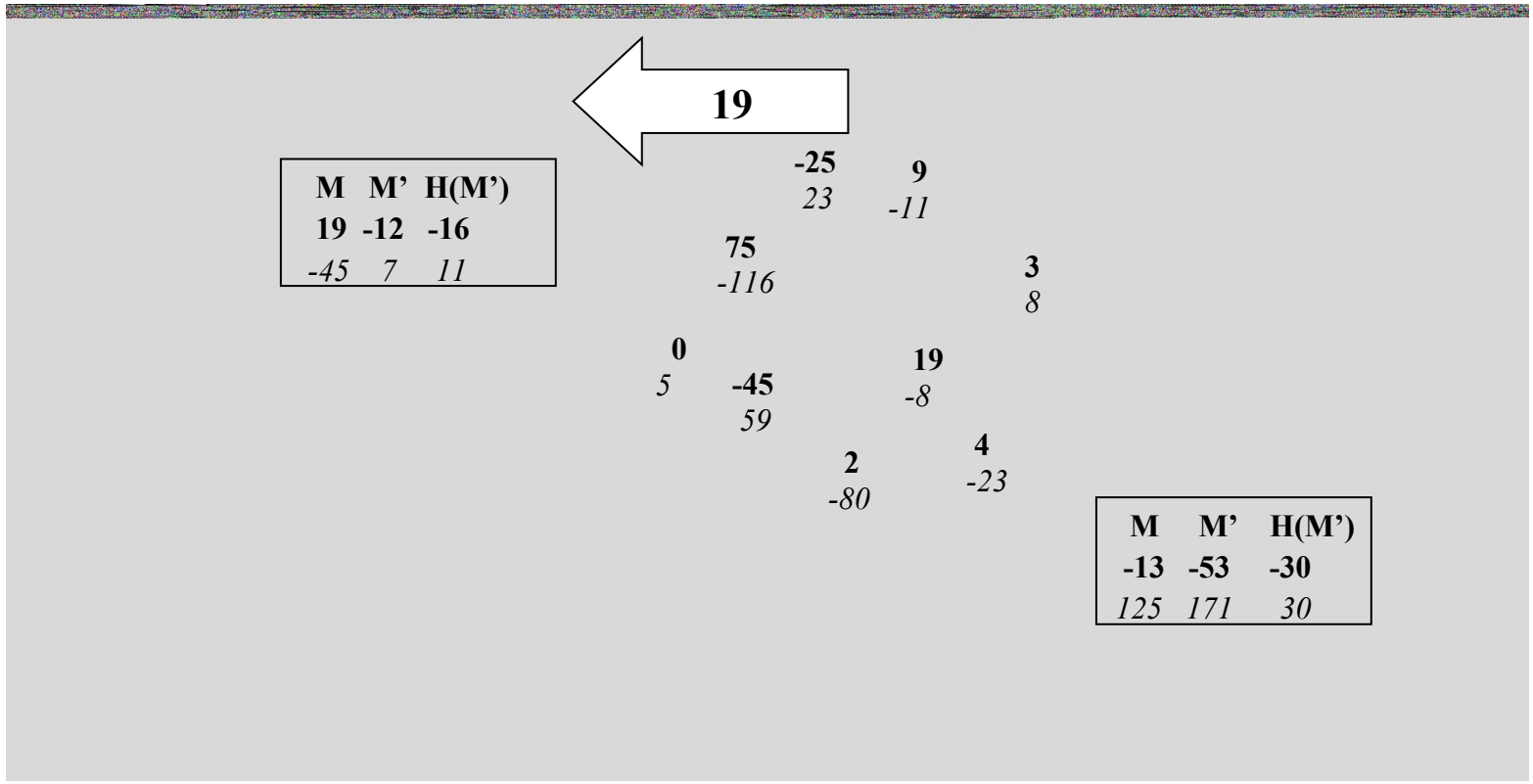
Supplementary Figure 23 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3), $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}), $\Delta_b^{CP}M(\Omega)$ (in au multiplied by 10^3), and $\Delta_b^{CP}v(\Omega)$ (in parenthesis and in au) in **HE1**. See supplementary material for corresponding values for the remaining complexes studied here in. Summation of these atomic variations (excluding $\Delta_b^{CP}M(\Omega)$) are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed or included in the methyl group attached to C3" (H(M')). The arrow indicates the total electron density transference between both monomers (in au multiplied by 10^3).



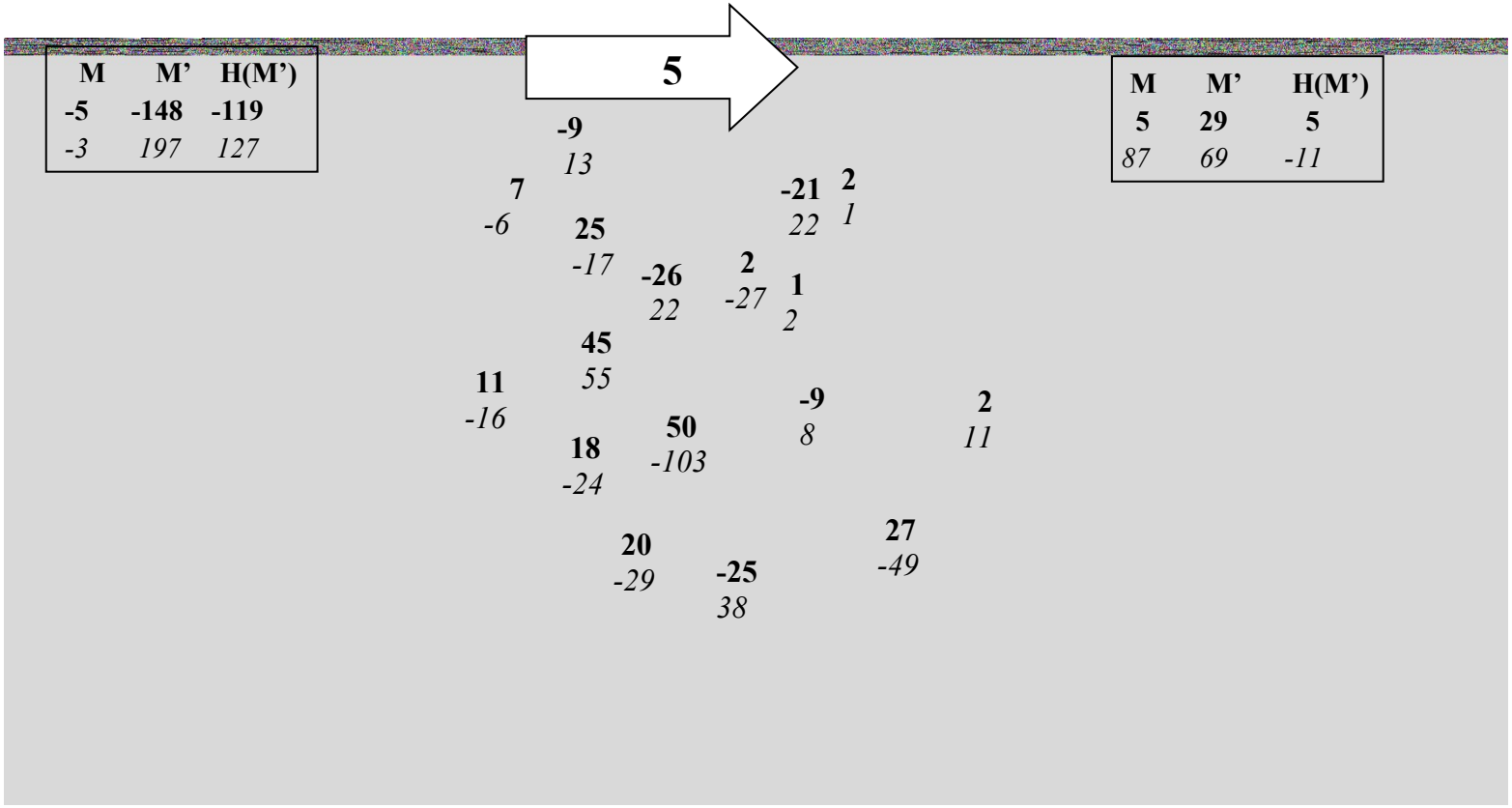
Supplementary Figure 24 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3) and $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}) in **HE2**. Summation of these atomic variations are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed or included in the methyl group attached to C2' (H(M')). The arrow indicates the total electron density transference between both monomers (in au multiplied by 10^3).



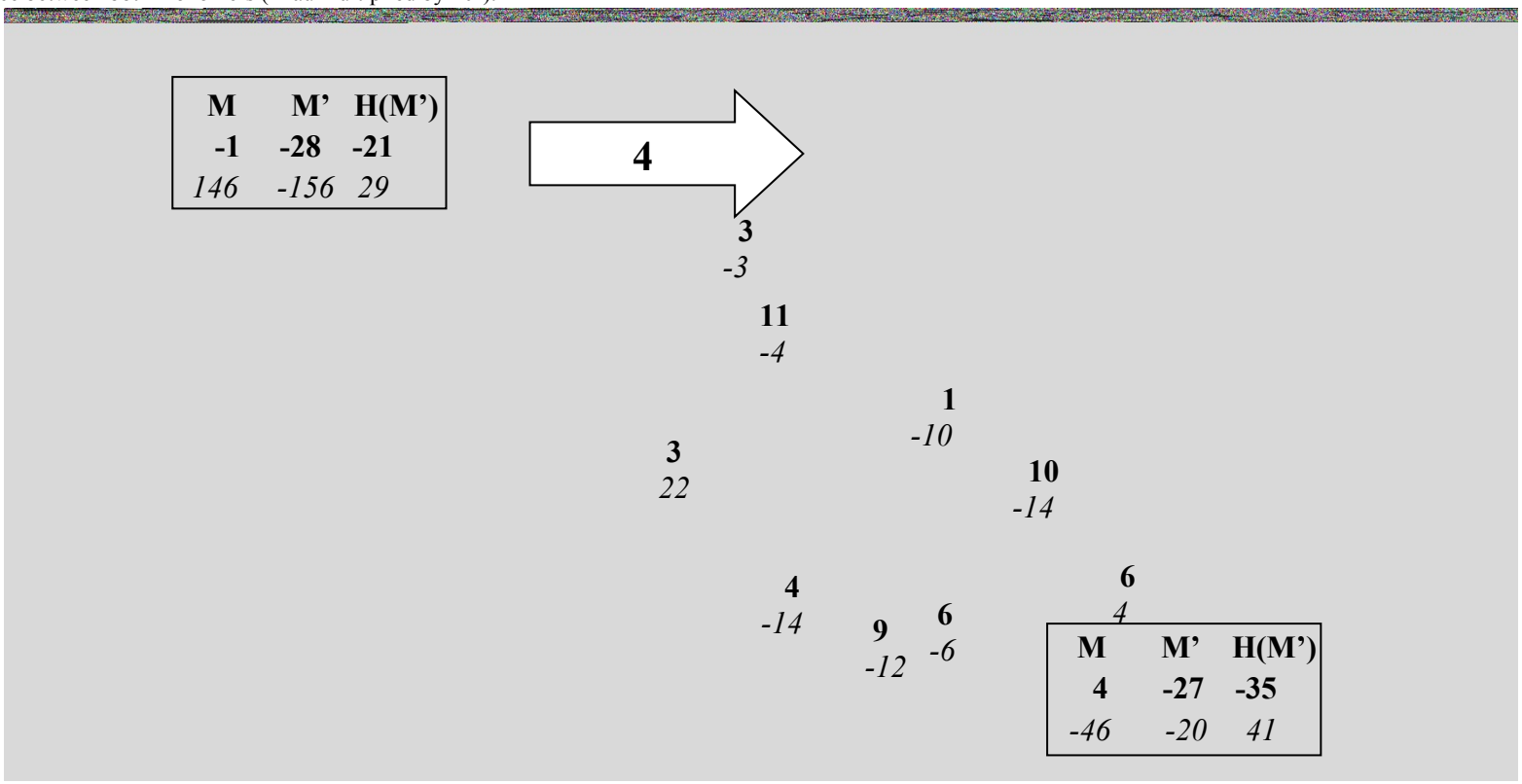
Supplementary Figure 25 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3) and $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}) in **MC1**. Summation of these atomic variations are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed (H(M')). The arrow indicates the total electron density transference between both monomers (in au multiplied by 10^3).



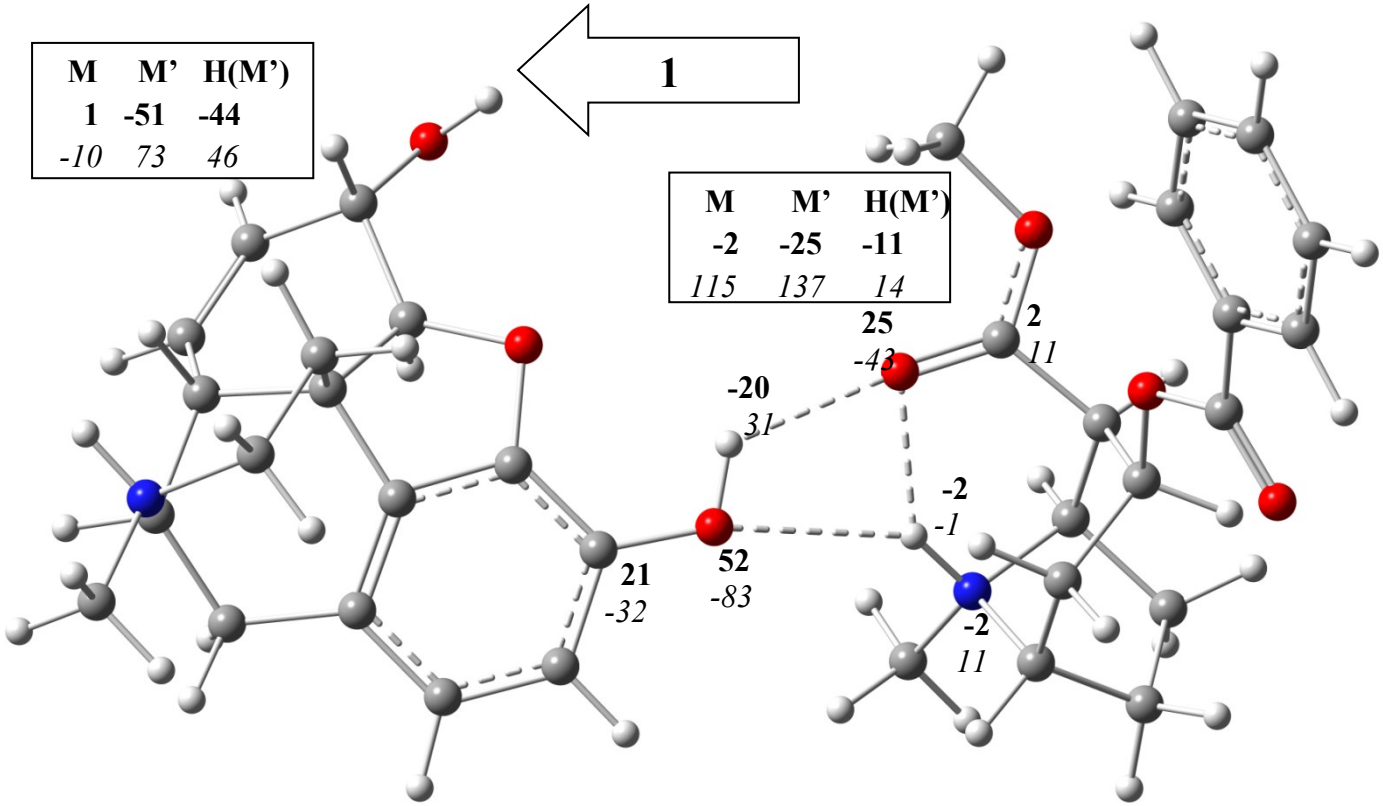
Supplementary Figure 26 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3) and $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}) in **MC2**. Summation of these atomic variations are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed (H(M')). The arrow indicates the total electron density transference between both monomers (in au multiplied by 10^3).



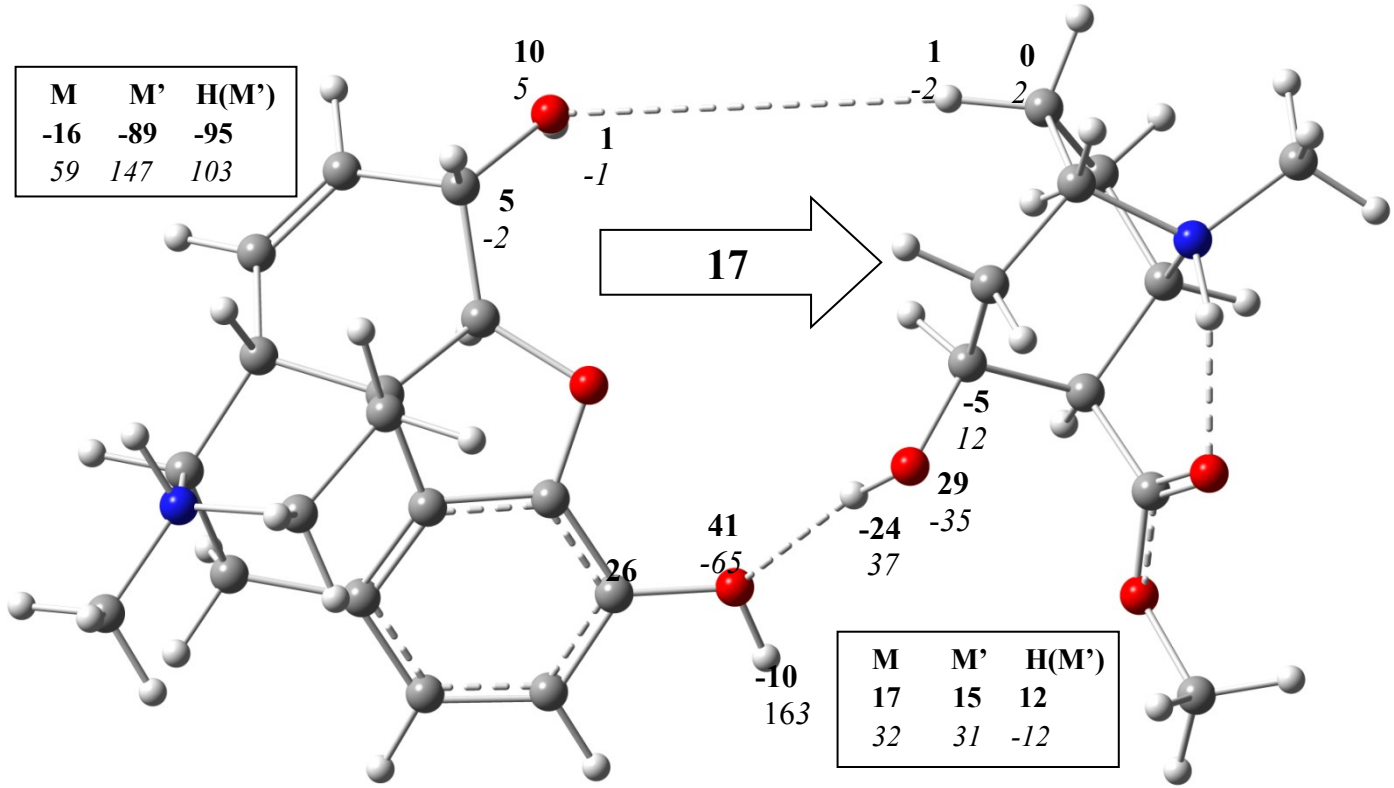
Supplementary Figure 27 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3) and $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}) in **MC3**. Summation of these atomic variations are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed (H(M')). The arrow indicates the total electron density transference between both monomers (in au multiplied by 10^3).



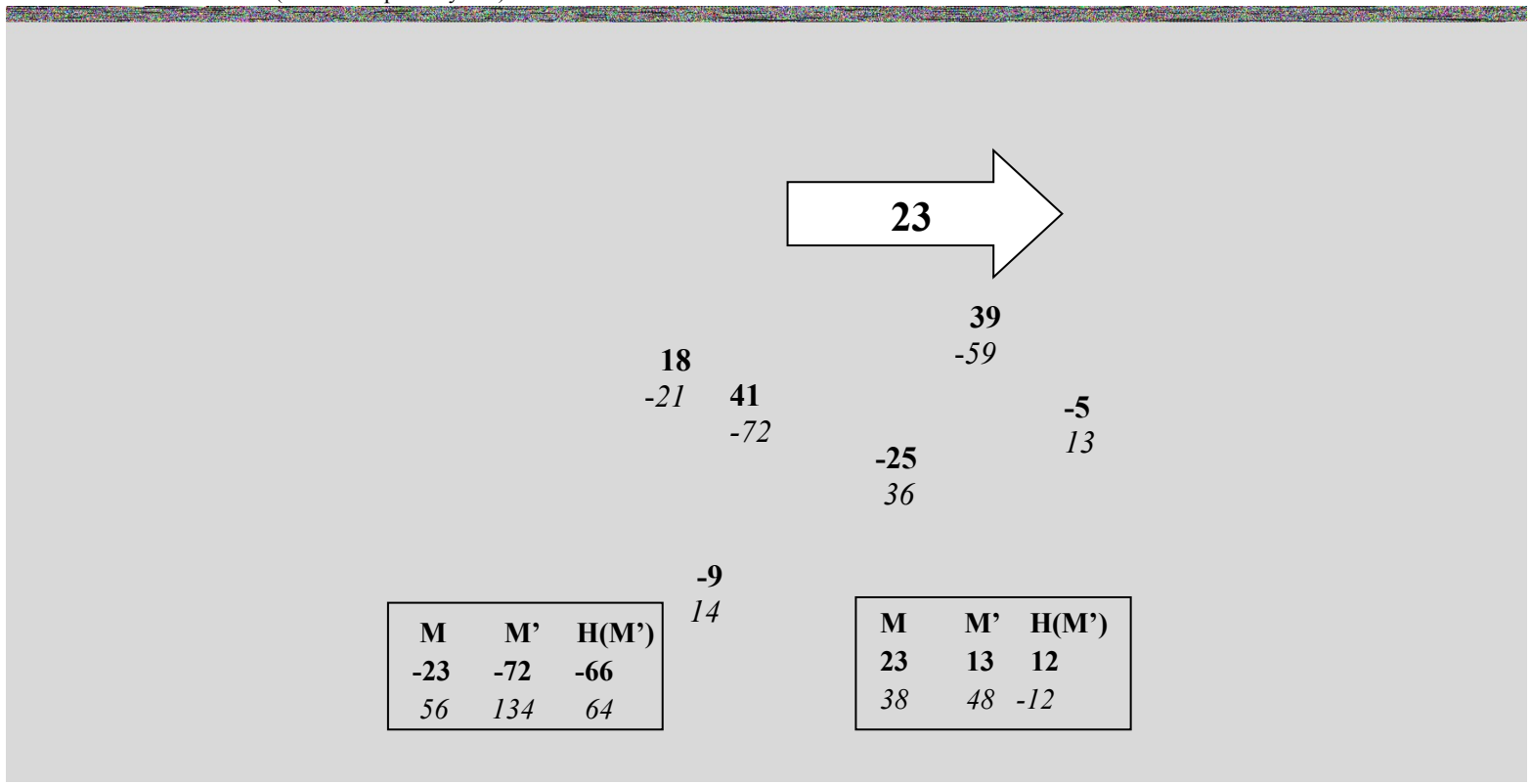
Supplementary Figure 28 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3) and $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}) in **MC4**. Summation of these atomic variations are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed (H(M')). The arrow indicates the total electron density transference between both monomers (in au multiplied by 10^3).



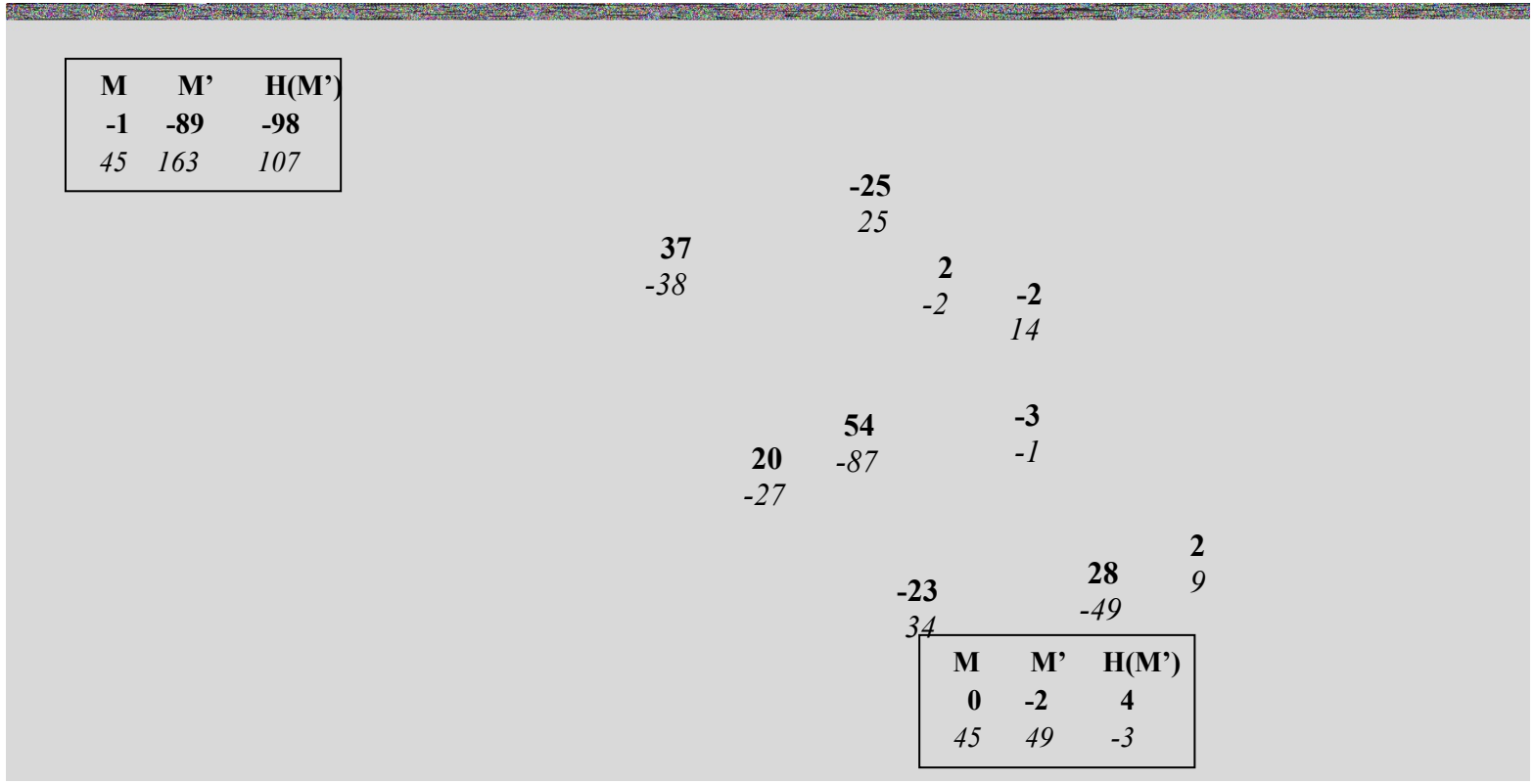
Supplementary Figure 29 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3) and $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}) in **ME1**. Summation of these atomic variations are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed (H(M')). The arrow indicates the total electron density transference between both monomers (in au multiplied by 10^3).



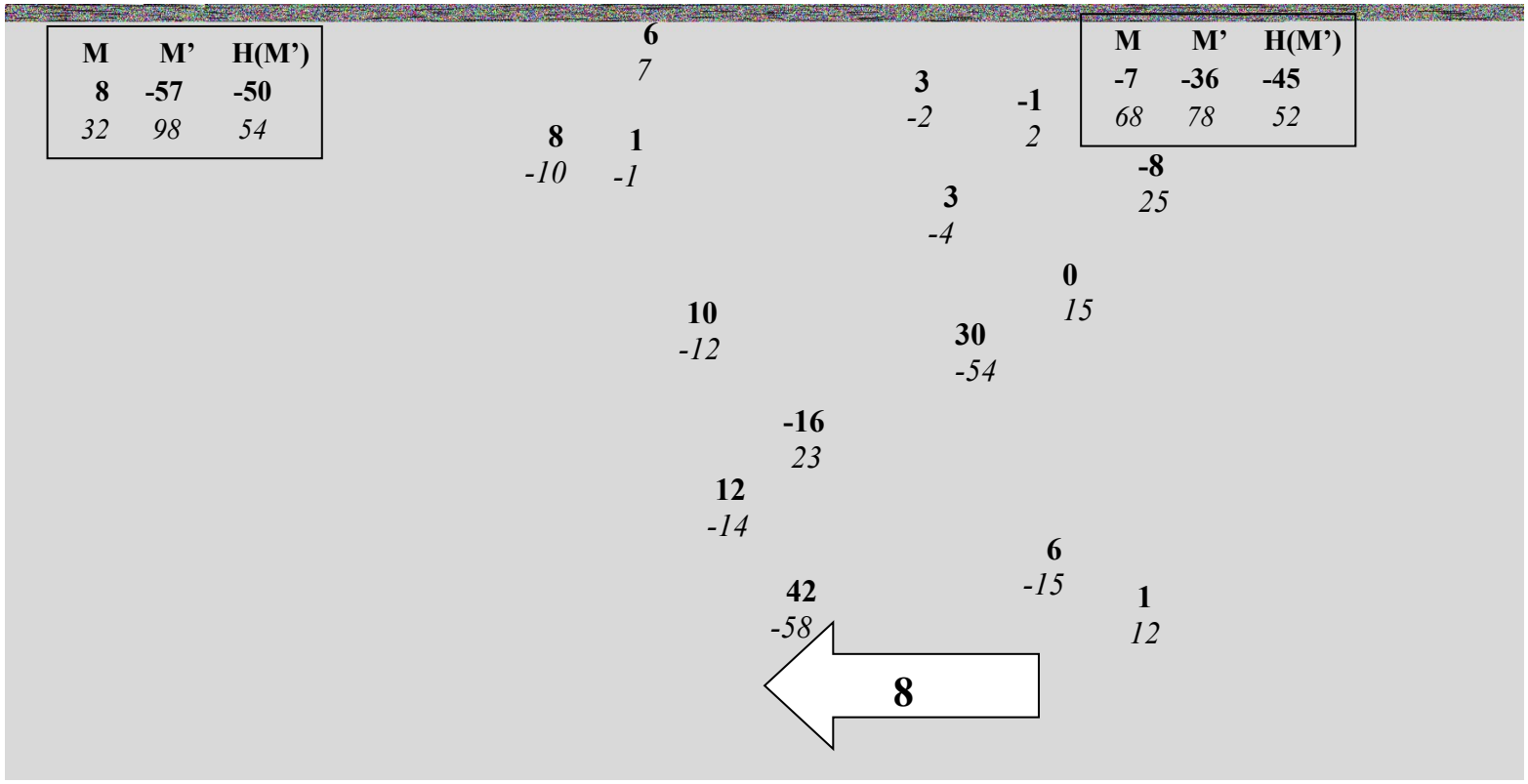
Supplementary Figure 30 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3) and $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}) in **ME2**. Summation of these atomic variations are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed (H(M')). The arrow indicates the total electron density transference between both monomers (in au multiplied by 10^3).



Supplementary Figure 31 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3) and $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}) in **ME3**. Summation of these atomic variations are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed (H(M')). In this case, we do not observe total electron density transference between both monomers.



Supplementary Figure 32 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3) and $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}) in **ME4**. Summation of these atomic variations are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed (H(M')). The arrow indicates the total electron density transference between both monomers (in au multiplied by 10^3).



Supplementary Figure 33 Most significant $\Delta_b^{CP}N(\Omega)$ (in boldface and in au and multiplied by 10^3) and $\Delta_b^{CP}E(\Omega)$ values (in italics and expressed in kJ mol^{-1}) in **ME5**. Summation of these atomic variations are shown for whole monomers (M), atoms and groups whose variation is not detailed (M'), and hydrogens not detailed (H(M' The arrow indicates the total electron density transference between both monomers (in au multiplied by 10^3).