Regioselectivity for Condensation Reactions of Quinonoid Models of Tryptophan Tryptophylquinone: A Density Functional Theory Study

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Table S1 The optimized geometries of **OBQ**, **MIQ**, **IIQ** at the B3LYP/D95(d,p) level (Bond distances in Å, angles in Deg., and E_{total} in a.u.).

Parameter	OBQ	MIQ	IIQ	
	B3LYP	B3LYP	B3LYP	Exp. ^a
N ₁ C ₂		1.367	1.366	1.370
N ₁ 'C ₂ '			1.397	1.371
N ₁ C ₈		1.371	1.370	1.377
N ₁ 'C ₈ '			1.380	1.377
C ₂ C ₃		1.400	1.400	1.362
C ₄ C ₂ '			1.468	1.498
C ₄ C ₅	1.356	1.364	1.370	1.388
C ₆ O ₁	1.221	1.224	1.225	1.241
C ₆ N ₂				
C ₇ O ₂	1.221	1.227	1.227	1.233
C ₇ N ₂				
C ₄ C ₉	1.468	1.471	1.475	1.422
C ₅ C ₆	1.480	1.476	1.473	1.402
C ₆ C ₇	1.566	1.563	1.560	1.380
C ₇ C ₈	1.480	1.450	1.451	1.390
C ₈ C ₉	1.356	1.400	1.403	1.416
O ₁₁ H				
O ₁₀ H				
∠ C ₂ N ₁ C ₈		109.1	109.1	108.1
∠ C ₉ C ₈ N ₁		108.5	108.5	109.1
∠ C ₃ 'C ₂ 'N ₁ '			109.2	111.7
∠ C ₅ C ₆ C ₇	117.2	118.0	117.9	120.0
∠ C ₆ C ₇ C ₈	117.2	113.4	113.5	118.8
∠ C ₇ C ₈ C ₉	120.6	125.9	126.2	122.5
∠ C ₅ C ₄ C ₉	122.3	119.2	119.3	119.6
∠ O ₁₀ C ₆ C ₇	120.1	119.3	119.5	119.6
∠ O ₁₁ C ₇ C ₆	120.1	122.2	122.3	122.3
∠ C ₆ N ₁₀ H				
∠ C ₇ N ₁₁ H				
χ ^b			49.6	51.6 ^c
E _{total}	-381.506571	-591.767942	-954.438925	

^a No experimental structure of **IIQ** is available. The data is the X-ray crystal structure of TTQ in MADH from Ref.10. ^b χ is a dihedral angle (∠C5C4C2'C3') of **IIQ**. ^c There are two TTQ cofactors per protein and another one with the dihedral angle 57.3°.

Table S2 Some structural parameters of **IIQ** scanned PES along the dihedral angle $C_5C_4C_2'C_3'$, χ , at the B3LYP/D95(d,p) level (Bond distances in Å, angles in Deg., and ΔE in kcal/mo)

χ	C ₆ O ₁₀	C ₇ O ₁₁	C ₄ C ₅	C ₄ C ₉	C ₅ C ₆	C ₆ C ₇	C ₄ C ₂ '	$\angle C_5C_4C_2'$	$\angle C_4C_2'C_3'$	$\angle C_9C_4C_2'$	$\angle C_4C_2'N_1'$	ΔE
0.0	1.228	1.227	1.378	1.492	1.465	1.551	1.459	120.6	131.4	121.8	119.2	5.30
5.0	1.228	1.227	1.377	1.490	1.466	1.552	1.460	120.5	131.4	121.6	119.1	4.35
10.0	1.228	1.227	1.377	1.488	1.466	1.553	1.460	120.4	131.4	121.5	119.2	3.45
30.0 ^a	1.227	1.227	1.374	1.481	1.469	1.556	1.462	119.7	130.8	121.4	120.0	0.81
49.6	1.225	1.227	1.370	1.475	1.473	1.560	1.468	119.4	130.4	121.2	120.4	0.00
70.0	1.224	1.228	1.366	1.472	1.478	1.563	1.477	119.9	130.3	120.5	120.1	0.56
80.0	1.223	1.227	1.365	1.470	1.480	1.564	1.482	120.1	130.2	120.2	119.9	1.07
90.0	1.223	1.227	1.364	1.469	1.482	1.565	1.485	120.3	130.3	120.1	119.7	1.52
100.0	1.223	1.227	1.364	1.468	1.481	1.565	1.485	119.8	130.4	120.6	119.9	1.70
120.0	1.225	1.227	1.371	1.472	1.474	1.560	1.474	118.8	130.9	121.8	119.4	0.78
123.5	1.226	1.227	1.372	1.473	1.473	1.560	1.472	118.7	131.1	122.0	119.3	0.74
130.0	1.226	1.228	1.373	1.474	1.472	1.558	1.470	118.6	131.4	122.3	119.3	0.88
140.0	1.227	1.228	1.375	1.477	1.470	1.556	1.467	118.3	132.1	122.8	119.0	1.60
150.0 ^b	1.227	1.228	1.377	1.480	1.468	1.555	1.465	118.2	132.7	123.4	118.7	2.99
180.0 ^c	1.227	1.227	1.380	1.489	1.468	1.554	1.464	119.2	133.8	124.3	117.5	11.32

^a There is that threshold has not yet satisfy default , i.e., maximum displacement = 0.002426 (Å).

^b There is that threshold has not yet satisfy default , i.e., maximum force = 0.002426 (Hartree/Bohr of radian).

^c There is that threshold has not yet satisfy default , i.e., maximum displacement = 0.002426 (Å).

Table S3 The calculated vibrational frequencies (in cm^{-1}) of the **OBQ**, **MIQ**, and **IIQ** at the B3LYP/D95(d,p) level scaled by 0.96 (predicted infrared intensities, in mDyne/A, are listed in parentheses).

OBQ			MIQ			IIQ	
normal mode	sym.	ν	normal mode	sym.	ν	normal mode	ν
CO asym-str	B ₂	1703 (65.6)	CO asym-str	A'	1689 (41.0)	CO asym-str	1683 (19.2)
CO sym-str	A ₁	1679 (220.4)	CO sym-str	A'	1665 (498.4)	CO sym-str	1658 (683.8)
C ₄ C ₅ , C ₈ C ₉ asym-str	B ₂	1606 (0.2)	C ₄ C ₅ str	A'	1580 (65.3)	C ₄ C ₅ str	1556 (158.5)
C ₄ C ₅ , C ₈ C ₉ sym-str	A ₁	1550 (2.2)	C ₄ C ₅ , C ₈ C ₉ sym-str	A'	1521 (14.9)	C ₂ 'C ₃ ' str	1526 (102.1)
			C ₂ C ₃ str	A'	1476 (37.8)	C ₄ C ₅ , C ₈ C ₉ sym-str	1508 (52.4)

Appendix 1

(Optimized Cartesian Coordinates and energies)

OBQ	(B3LYP/D95(d,p) E= -381.506571 a.u.		
C	0.783111	0.000000	0.677260
C	1.458395	0.000000	-0.639377
C	0.734177	0.000000	-1.785809
C	-0.734177	0.000000	-1.785809
C	-1.458395	0.000000	-0.639377
C	-0.783111	0.000000	0.677260
O	1.395093	0.000000	1.734282
H	2.546090	0.000000	-0.636468
H	1.239943	0.000000	-2.750237
H	-1.239943	0.000000	-2.750237
H	-2.546090	0.000000	-0.636468
O	-1.395093	0.000000	1.734282
MIQ	(B3LYP/D95(d,p) E= -591.767942 a.u.		
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.476230
C	1.381015	0.000000	-0.733182
O	-1.030178	-0.000000	-0.661478
C	1.131966	0.000000	2.236958
C	2.513269	0.000000	0.172524
H	-0.984128	-0.000000	1.938995
O	1.471111	-0.000000	-1.957048
C	2.444628	0.000000	1.572207
N	3.833377	-0.000000	-0.198730
C	1.047906	0.000000	3.741328
C	3.793072	-0.000000	2.057394
C	4.613054	0.000000	0.924076
H	4.142425	-0.000000	-1.162702
H	1.546598	0.881779	4.162132
H	1.546598	-0.881779	4.162132
H	0.007192	0.000000	4.075673
H	5.693643	-0.000000	0.863872

C	4.314499	-0.000000	3.470071
H	5.409306	-0.000000	3.472147
H	3.983164	-0.883916	4.027348
H	3.983164	0.883916	4.027348

IIQ (B3LYP/D95(d,p) E= -954.438925 a.u.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.473080
C	1.379155	0.000000	-0.728671
O	-1.032084	0.032256	-0.660060
C	1.135928	-0.010105	2.239434
C	2.511914	-0.040365	0.176931
H	-0.977619	0.086689	1.938151
O	1.474402	0.001207	-1.952358
C	2.452630	-0.084417	1.577952
C	1.021556	0.080368	3.700221
N	3.820083	-0.179194	-0.207737
C	3.793812	-0.288395	2.047075
C	4.599430	-0.331600	0.903334
H	4.115358	-0.201229	-1.175958
C	0.229740	-0.639011	4.588395
N	1.764469	1.026963	4.409931
C	4.324144	-0.495591	3.441891
H	5.669627	-0.475442	0.829883
C	-0.684512	-1.792768	4.288618
H	2.292913	1.769565	3.975436
C	0.495056	-0.100413	5.899419
C	1.440261	0.955178	5.749657
C	1.892727	1.716330	6.838866
C	0.011671	-0.412870	7.188464
H	4.411953	0.442190	4.002070
H	5.320051	-0.949170	3.400423
H	3.674125	-1.156433	4.023606
H	-0.576153	-2.134316	3.255699
H	-0.473179	-2.640342	4.952584
H	-1.736494	-1.516830	4.440221
H	2.608469	2.525998	6.711124
C	1.391243	1.390865	8.101191

C	0.462177	0.335042	8.275649
H	-0.707263	-1.217022	7.331084
H	1.721994	1.958050	8.968797
H	0.096395	0.111550	9.275539

IIQ'   B3LYP/D95(d,p)   E= -954.4377442 a.u.

C	2.656456	-2.070055	0.242502
C	1.221255	-1.749721	0.154767
C	3.671922	-0.889153	0.158658
O	3.068834	-3.212816	0.403734
C	0.726115	-0.478634	0.009676
C	3.041396	0.400882	-0.046794
H	0.550148	-2.591560	0.304042
O	4.885251	-1.062813	0.223222
C	1.664374	0.642948	-0.165737
C	-0.732924	-0.282749	0.011411
N	3.711494	1.568019	-0.305129
C	1.512273	2.017855	-0.546531
C	2.807006	2.545022	-0.610797
H	4.721242	1.641799	-0.301158
C	-1.546909	0.512352	0.808735
N	-1.534282	-1.099587	-0.789559
C	0.276825	2.806234	-0.890665
H	3.121366	3.548561	-0.866557
C	-1.135075	1.420716	1.932005
H	-1.174756	-1.690462	-1.525745
C	-2.906554	0.191494	0.453460
C	-2.863265	-0.805034	-0.564436
C	-4.026038	-1.322344	-1.156856
C	-4.160108	0.656248	0.908028
H	-0.403984	2.227955	-1.522593
H	0.551169	3.719458	-1.429440
H	-0.284364	3.102118	0.001205
H	-0.050794	1.554641	1.972017
H	-1.601502	2.409939	1.837946
H	-1.453220	1.007869	2.898293
H	-3.980014	-2.078061	-1.938365
C	-5.251228	-0.836904	-0.695381

C	-5.318785	0.140468	0.329138
H	-4.222349	1.406273	1.693942
H	-6.173313	-1.219820	-1.127748
H	-6.293199	0.489541	0.664221

IIQ-TS   B3LYP/D95(d,p)   E= -954.436203 a.u.

C	2.842975	-1.950680	.001038
C	1.373901	-1.759249	.041894
C	3.751465	-.679314	-.090836
O	3.358081	-3.059094	.038944
C	.776694	-.533809	.001863
C	3.002560	.559696	-.134167
O	4.975556	-.758998	-.128201
C	1.605381	.674318	-.101265
C	-.704731	-.427743	.041544
N	3.534412	1.819718	-.240914
C	1.289466	2.066968	-.197715
C	2.517320	2.733139	-.281404
C	-1.554923	-.169686	1.098127
N	-1.444695	-.579380	-1.130717
C	-.054028	2.743887	-.213797
C	-1.176596	.064563	2.532771
C	-2.893865	-.170752	.553316
C	-2.789630	-.434538	-.842781
C	-3.914327	-.511332	-1.678483
C	-4.170869	.023929	1.120014
C	-5.166460	-.315693	-1.090287
C	-5.293903	-.049423	.294648
H	.782465	-2.667328	.125746
H	4.528466	2.005408	-.287810
H	2.713325	3.794107	-.367000
H	-1.052488	-.835812	-2.025014
H	-.706282	2.327214	-.988767
H	.060146	3.816078	-.404968
H	-.576459	2.622845	.741276
H	-.093954	-.005778	2.676178
H	-1.498706	1.056735	2.876942
H	-1.648755	-.674435	3.192659

H	-3.820704	-.717381	-2.742989
H	-4.280440	.226131	2.183701
H	-6.060471	-.369232	-1.708118
H	-6.285841	.098131	.716756

Carbinolamine intermediates

6MIQ-I	(B3LYP/D95++(d,p))		E= -648.36742 a.u.
C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.514580
C	1.403143	0.000000	-0.657737
O	-0.675643	1.199037	-0.410847
N	-0.624535	-1.227427	-0.469023
C	1.096275	-0.129754	2.291366
C	2.505539	-0.172965	0.240578
H	-0.984355	0.105359	1.968937
O	1.492857	0.139630	-1.885173
H	-0.467646	1.319140	-1.353941
H	-1.591400	-1.278388	-0.153306
H	-0.602639	-1.264626	-1.488371
C	2.412122	-0.240507	1.639820
C	0.989416	-0.144945	3.797960
N	3.831148	-0.263797	-0.116372
C	3.746503	-0.386354	2.136953
C	4.581000	-0.397742	1.015837
H	4.160434	-0.238573	-1.072504
H	1.563257	0.674502	4.248392
H	1.377446	-1.081582	4.217297
H	-0.053747	-0.040010	4.110970
C	4.244295	-0.510709	3.553660
H	5.658849	-0.493325	0.970071
H	3.989504	0.367975	4.157952
H	5.334923	-0.612692	3.564453
H	3.826310	-1.389311	4.059324
7MIQ-I	(B3LYP/D95++(d,p))		E= -648.36542 a.u.
C	0.000000	0.000000	0.000000

C	0.000000	0.000000	1.451840
C	1.360616	0.000000	-0.758716
O	-1.015390	-0.038742	-0.703177
C	1.126964	0.238827	2.197838
C	2.471726	0.430504	0.146542
H	-0.966020	-0.141742	1.930515
N	1.549525	-1.396907	-1.131566
O	1.291675	0.901609	-1.863307
C	2.397930	0.502160	1.533823
C	1.039738	0.261473	3.701717
N	3.734966	0.753890	-0.242137
H	0.760857	-1.715134	-1.694722
H	2.410130	-1.521653	-1.661530
H	0.375657	0.841822	-2.192117
C	3.710868	0.892705	2.006897
C	4.496278	1.045136	0.879707
H	4.024839	0.875832	-1.203168
H	1.334755	1.240850	4.097829
H	1.720578	-0.478445	4.140748
H	0.023626	0.042622	4.040836
C	4.194248	1.123217	3.413873
H	5.531609	1.346293	0.789966
H	3.637872	1.925991	3.913783
H	5.251249	1.410360	3.407838
H	4.100131	0.223774	4.034929

6IIQ-I (B3LYP/D95(d,p) E= -1011.02145 a.u.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.550000
C	1.373526	0.000000	2.191624
C	2.534183	-0.194603	1.524081
C	2.492000	-0.380624	0.063483
C	1.267743	-0.260461	-0.615206
N	1.493739	-0.453911	-1.958663
C	3.487625	-0.685061	-0.916797
C	2.820417	-0.719130	-2.147184
C	3.821977	-0.188381	2.253430
N	4.749311	0.831742	2.027584

C	4.330259	-1.073234	3.186904
C	5.632639	-0.569831	3.562816
C	5.853971	0.635689	2.836274
C	7.021775	1.398742	2.985919
C	6.625104	-1.021270	4.456860
C	7.984670	0.933174	3.886188
C	7.795634	-0.274330	4.600931
N	-0.679552	-1.235733	1.916090
O	-0.656300	1.191882	1.993225
O	-1.067646	0.188370	-0.599809
H	-1.586707	-1.278984	1.451765
H	-0.827414	-1.267112	2.922805
H	-1.396576	1.329485	1.376957
H	1.386364	0.174785	3.265416
H	0.766520	-0.431567	-2.660641
H	3.220851	-0.923668	-3.132428
C	4.957138	-0.956634	-0.738455
C	3.694392	-2.338263	3.688280
H	6.483324	-1.938306	5.024916
H	8.570568	-0.609875	5.286957
H	8.902472	1.500240	4.026955
H	7.177654	2.317598	2.424538
H	4.548269	1.669437	1.500376
H	5.514235	-0.052424	-0.467784
H	5.387414	-1.353024	-1.664070
H	5.132327	-1.687103	0.058255
H	2.733663	-2.519033	3.197203
H	4.339486	-3.207358	3.503526
H	3.516397	-2.292807	4.770803

7IIQ-I (B3LYP/D95(d,p)) E= -1011.01782 a.u.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.552000
C	1.264193	0.000000	2.264191
C	2.471129	0.244299	1.643493
C	2.527488	0.452711	0.197522
C	1.339728	0.402473	-0.533060
N	1.626213	0.604000	-1.847181

C	3.599995	0.672509	-0.757792
C	2.993459	0.775045	-1.996782
C	3.673295	0.354451	2.485781
N	4.482063	1.490476	2.421305
C	4.182144	-0.516435	3.440743
C	5.357195	0.118763	3.986664
C	5.503168	1.381779	3.343221
C	6.539394	2.272299	3.666374
C	6.295208	-0.263817	4.968848
C	7.448718	1.870535	4.647865
C	7.331129	0.613677	5.289623
N	-0.240853	-1.398905	-0.341549
O	-0.989210	0.906317	-0.480290
O	-1.109293	-0.004403	2.099374
H	-1.114471	-1.707919	0.084716
H	-0.306013	-1.520359	-1.350175
H	-1.709631	0.862070	0.175195
H	1.206836	-0.066247	3.346650
H	0.931100	0.707197	-2.574016
H	3.434983	0.949622	-2.969047
C	5.091903	0.729665	-0.552858
C	3.673232	-1.879585	3.813347
H	6.206813	-1.222682	5.475314
H	8.063043	0.334458	6.044661
H	8.264436	2.535685	4.923410
H	6.640548	3.234152	3.168026
H	4.247820	2.320288	1.897260
H	5.425839	1.681623	-0.124514
H	5.603833	0.604515	-1.512697
H	5.436683	-0.062564	0.119841
H	2.846696	-2.189205	3.168659
H	4.469847	-2.630651	3.730240
H	3.315639	-1.899940	4.851284

1	(B3LYP/D95++(d,p))		E= -609.04236 a.u.
C	-1.660549	0.238000	0.023941
C	-0.841590	1.510510	-0.058952
C	-0.859742	-1.097609	-0.072037

O	-2.581502	0.276860	-1.073477
N	-2.293665	0.186628	1.333930
C	0.507347	1.541286	-0.042265
C	0.580023	-1.001235	0.001048
H	-1.417473	2.432873	-0.120305
O	-1.512434	-2.137324	-0.194357
H	-2.905817	-0.635100	-1.181741
H	-2.939155	0.966474	1.447111
H	-2.809531	-0.687967	1.435118
C	1.195483	0.257882	0.011921
C	1.311111	2.817663	-0.088123
C	1.610727	-1.995101	0.019531
N	2.547417	0.045270	0.043315
C	2.812234	-1.320235	0.050324
H	1.976972	2.841533	-0.962068
H	1.935431	2.929297	0.809613
H	0.653192	3.689282	-0.145846
H	1.471969	-3.068025	0.015740
H	3.829628	-1.686978	0.080470
H	3.249753	0.772067	0.051549

2	(B3LYP/D95++(d,p))		E= -609.04105 a.u.
C	-1.519446	0.927065	-0.110966
C	-0.427567	1.888799	-0.015038
C	-1.236844	-0.599353	0.056639
O	-2.695787	1.252489	-0.300412
C	0.885559	1.501274	0.027053
C	0.228699	-0.924380	-0.032129
H	-0.705204	2.939824	-0.038971
N	-1.709740	-0.887664	1.405383
O	-1.927056	-1.303234	-0.975738
C	1.181413	0.088608	0.000402
C	2.012272	2.500856	0.075390
C	0.911846	-2.164178	-0.098933
H	-2.697054	-0.644496	1.487141
H	-1.586984	-1.874801	1.623278
H	-2.771156	-0.831937	-1.096045
N	2.429274	-0.512407	-0.041840

C	2.273682	-1.875415	-0.104903
H	0.474423	-3.152335	-0.160841
H	2.669132	2.397001	-0.799308
H	2.629242	2.351616	0.972039
H	1.631040	3.524987	0.091866
H	3.129789	-2.535449	-0.155838
H	3.315098	-0.027608	-0.044015

3 (B3LYP/D95++(d,p)) E= -625.09605 a.u.

C	-1.640928	0.242274	0.015623
C	-0.817223	1.517178	-0.052543
C	-0.840143	-1.090120	-0.057366
O	-2.532919	0.276367	-1.106337
N	-2.300612	0.188919	1.310118
C	0.531397	1.567611	-0.032984
C	0.584062	-0.936070	0.012519
H	-1.403945	2.432972	-0.110343
O	-1.452371	-2.157965	-0.162104
H	-2.894458	-0.622396	-1.199262
H	-2.914508	0.991463	1.435688
H	-2.845291	-0.669332	1.395946
C	1.245972	0.291049	0.016108
C	1.328876	2.844311	-0.070724
N	1.581715	-1.894192	0.020190
N	2.605209	0.098752	0.035745
C	2.765161	-1.221204	0.039954
H	1.436766	-2.896216	0.017929
H	2.006345	2.853043	-0.933129
H	1.958268	2.932861	0.823328
H	0.670618	3.716476	-0.127712
H	3.721287	-1.730611	0.059197

4 (B3LYP/D95++(d,p)) E= -625.09549 a.u.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.457400
C	1.352231	0.000000	-0.790620
O	-1.021283	-0.026852	-0.692467
C	1.133915	0.203151	2.198190

C	2.480479	0.357440	0.122954
H	-0.970825	-0.112993	1.933795
N	1.495542	-1.374546	-1.245396
O	1.287879	0.970069	-1.835204
C	2.392431	0.413447	1.498117
C	1.129435	0.251002	3.698120
N	3.787074	0.643695	-0.176982
H	0.666675	-1.653840	-1.770157
H	2.316552	-1.482386	-1.838228
H	0.373963	0.936205	-2.172616
N	3.623228	0.727933	2.052404
C	4.432533	0.864912	1.022883
H	4.175291	0.762583	-1.104074
H	1.526518	1.211955	4.047210
H	1.798534	-0.520071	4.100115
H	0.124219	0.103997	4.102144
H	5.482790	1.124242	1.071659

5 (B3LYP/D95++(d,p)) E= -647.14632 a.u.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.508500
C	1.420282	0.000000	-0.610415
O	-0.693929	1.166806	-0.427894
N	-0.574918	-1.256867	-0.474811
C	1.060308	-0.351039	2.260194
C	2.526148	-0.581052	0.213569
H	-0.940519	0.293339	1.972502
O	1.569903	0.443891	-1.738311
H	-0.342351	1.383110	-1.310649
H	-0.636198	-1.252454	-1.493259
H	-1.510724	-1.385704	-0.093474
C	2.336803	-0.729650	1.611677
C	0.971867	-0.374106	3.768527
N	3.663011	-0.883172	-0.430909
H	1.729915	0.273847	4.227534
H	1.123823	-1.387274	4.164054
H	-0.012188	-0.030354	4.099331
C	4.678487	-1.369377	0.286473

C	3.433809	-1.221768	2.343232
C	4.613612	-1.551851	1.677254
H	3.365190	-1.348194	3.419764
H	5.584485	-1.621409	-0.264463
H	5.472873	-1.940406	2.218672

6 (B3LYP/D95++(d,p)) E= -647.15584 a.u.

C	1.934293	0.480992	-0.017252
C	1.203708	1.742788	-0.054298
C	1.155259	-0.853003	-0.002398
O	3.163999	0.421722	0.042182
C	-0.154730	1.807065	-0.024659
C	-0.360964	-0.696806	0.004058
H	1.810993	2.644945	-0.072520
N	1.528569	-1.556195	-1.206292
O	1.492423	-1.510988	1.228851
C	-0.971387	0.578058	0.006054
C	-0.847793	3.145939	-0.027708
N	-1.047064	-1.843372	-0.013262
H	2.541167	-1.651662	-1.265758
H	1.080538	-2.470854	-1.223590
H	2.455223	-1.417147	1.330176
C	-2.384289	-1.786521	0.000293
H	-1.470120	3.271400	0.867837
H	-1.507810	3.247508	-0.898980
H	-0.119561	3.960230	-0.054228
C	-2.378260	0.612533	0.024748
H	-2.908146	-2.742241	-0.013939
C	-3.097955	-0.582127	0.028559
H	-2.906790	1.561395	0.031558
H	-4.184698	-0.585976	0.043684

7 (B3LYP/D95++(d,p)) E= -647.15548 a.u.

C	-1.896315	0.016608	0.057983
C	-1.299717	1.396681	-0.066306
C	-0.874776	-1.125474	-0.135361
O	-2.907336	-0.093349	-0.944738
N	-2.371972	-0.172303	1.422947

C	0.020780	1.660896	-0.077277
C	0.563087	-0.803092	-0.034361
H	-2.025876	2.206015	-0.131688
O	-1.302496	-2.258706	-0.340168
H	-3.070690	-1.044728	-1.069224
H	-2.814169	-1.086399	1.520512
H	-3.045371	0.550187	1.671671
C	0.995593	0.547375	-0.009968
C	0.558927	3.066773	-0.157875
C	1.518352	-1.827523	-0.009125
H	1.213926	3.186336	-1.028396
H	1.169543	3.299515	0.721960
H	-0.260659	3.788720	-0.225373
C	2.867725	-1.485762	0.063026
N	2.302830	0.870541	0.047808
H	1.184482	-2.861766	-0.042334
C	3.199515	-0.121748	0.090115
H	3.647623	-2.241703	0.096096
H	4.244821	0.184190	0.145619

8 (B3LYP/D95++(d,p)) E= -647.15880 a.u.

C	-1.910603	0.511116	-0.194466
C	-1.160302	1.755239	-0.079875
C	-1.187016	-0.824304	0.103846
O	-3.110935	0.456303	-0.466540
C	0.196534	1.779572	0.022183
C	0.322504	-0.732121	-0.017668
H	-1.739476	2.674461	-0.133606
N	-1.512194	-1.083566	1.503424
O	-1.652731	-1.816107	-0.805222
C	0.975318	0.517952	0.005335
C	0.953949	3.074228	0.104026
C	1.101920	-1.887287	-0.110045
H	-2.523340	-1.143253	1.622609
H	-1.089698	-1.956083	1.815323
H	-2.585245	-1.594041	-0.981413
C	2.493904	-1.765350	-0.147911
H	1.645227	3.169278	-0.741055

H	1.576645	3.094364	1.006034
H	0.270219	3.927518	0.114023
N	2.318345	0.635123	-0.020123
H	0.621428	-2.860552	-0.171890
H	3.135713	-2.639330	-0.224686
C	3.050853	-0.480518	-0.087362
H	4.132445	-0.345993	-0.102724

9 (B3LYP/D95++(d,p)) E= -663.18811 a.u.

C	-1.881011	-0.008679	0.110875
C	-1.316993	1.381659	-0.069980
C	-0.867751	-1.123313	-0.233449
O	-3.017317	-0.122756	-0.734937
N	-2.147468	-0.231115	1.529947
C	-0.000557	1.661957	-0.116537
C	0.587718	-0.794278	-0.059534
H	-2.059542	2.174438	-0.145489
O	-1.274968	-2.211753	-0.600480
H	-3.109774	-1.068369	-0.949999
H	-2.604470	-1.132495	1.668942
H	-2.749044	0.501502	1.902364
C	0.982795	0.561485	-0.029672
C	0.500148	3.081161	-0.248132
N	1.457711	-1.810042	0.002598
H	1.142421	3.201756	-1.130123
H	1.089538	3.380208	0.628703
H	-0.338809	3.776285	-0.341700
C	2.747333	-1.477529	0.110870
C	2.373871	0.767275	0.057324
N	3.256225	-0.234702	0.134512
H	2.789082	1.773330	0.067899
H	3.460289	-2.297994	0.182758

10 (B3LYP/D95++(d,p)) E= -663.20000 a.u.

C	-1.915267	0.519180	0.010773
C	-1.153833	1.764895	0.048821
C	-1.172429	-0.837859	0.003806
O	-3.144807	0.489611	-0.052050

C	0.205430	1.799702	0.023128
C	0.345285	-0.711412	-0.006425
H	-1.741026	2.680252	0.065729
N	-1.549273	-1.516428	1.219143
O	-1.520931	-1.500572	-1.217714
C	0.980962	0.546789	-0.006770
C	0.940222	3.115441	0.028294
N	1.034448	-1.855707	0.006733
H	-2.563182	-1.569371	1.302857
H	-1.137656	-2.447882	1.242722
H	-2.480181	-1.382580	-1.328042
C	2.368919	-1.757116	-0.006193
H	1.567505	3.221286	-0.866254
H	1.603072	3.194005	0.899722
H	0.238049	3.952240	0.055249
C	2.386861	0.510960	-0.023084
H	2.926943	-2.692893	0.002653
N	3.089978	-0.628032	-0.028872
H	2.969411	1.430313	-0.029631

11 (B3LYP/D95++(d,p)) E= -739.43816 a.u.

C	2.968439	-1.910633	-0.019750
N	2.967880	-0.545325	-0.046121
C	1.664907	-0.096345	-0.039024
C	0.816506	-1.208078	-0.004024
C	1.649712	-2.361042	0.007530
C	-0.634653	-1.036631	0.012087
C	-1.170988	0.272170	0.001484
C	1.243496	1.276954	-0.027315
C	-0.286407	1.527521	0.008566
N	-2.483750	0.521428	-0.030368
C	-1.540064	-2.109946	0.019224
C	-2.910248	-1.849160	0.008184
N	-0.598857	2.303399	-1.166382
H	3.893093	-2.473622	-0.023025
H	1.347062	-3.399864	0.032949
H	-1.173128	-3.133861	0.028896
H	-3.638813	-2.655758	0.014909

O	2.010662	2.246345	-0.000174
O	-0.549846	2.178143	1.265741
H	-0.027147	3.145536	-1.204295
H	-1.589653	2.539810	-1.166252
H	0.118997	2.877920	1.356518
C	-3.332693	-0.513657	-0.025077
H	3.772292	0.068361	-0.064891
H	-4.394186	-0.267864	-0.050563

12 (B3LYP/D95++(d,p)) E= -739.42523 a.u.

C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.383047
C	1.292230	0.000000	1.833361
C	2.141553	-0.011266	0.739997
C	1.313282	-0.018689	-0.432196
C	3.589065	0.007415	0.924485
C	4.126885	0.202395	2.225910
C	1.725300	-0.060782	3.264195
C	3.203369	0.414818	3.390532
N	5.441554	0.260567	2.492053
C	4.510642	-0.120262	-0.130802
C	5.874435	-0.073773	0.145942
O	3.545537	0.905740	4.455069
N	1.779292	-1.451577	3.708728
O	0.881869	0.775036	4.046988
H	-0.925547	0.024011	-0.559309
H	1.631328	-0.016714	-1.467060
H	4.156494	-0.261315	-1.149296
H	6.611084	-0.177742	-0.647285
H	0.878002	-1.909157	3.586235
H	2.042661	-1.497458	4.692826
H	1.439729	1.111630	4.773110
C	6.293222	0.114046	1.475969
H	-0.810185	0.107489	1.978731
H	7.354213	0.149651	1.722493

13 (B3LYP/D95++(d,p)) E= -755.48267 a.u.

C	0.000000	0.000000	0.000000

N	0.000000	0.000000	1.365280
C	1.302129	0.000000	1.815345
C	2.149364	0.003797	0.701520
C	1.318701	0.003227	-0.451976
C	3.597215	0.006948	0.883245
C	4.133533	0.016392	2.188079
C	1.723648	0.030671	3.189361
C	3.254529	0.049222	3.445473
N	5.451152	-0.021077	2.406458
C	4.533366	-0.014843	-0.162262
N	5.855276	-0.032129	0.046176
N	3.552815	-1.125961	4.224015
H	-0.924470	-0.002683	-0.563175
H	1.622602	0.005272	-1.490566
H	4.205343	-0.018699	-1.201493
O	0.957693	0.082636	4.157694
O	3.542268	1.306338	4.078924
H	2.965988	-1.167458	5.055386
H	4.539352	-1.134668	4.477055
H	2.872666	1.424166	4.773968
C	6.244578	-0.042319	1.328679
H	-0.805604	0.001960	1.977998
H	7.317746	-0.070071	1.513984

14 (B3LYP/D95++(d,p)) E= -755.46699 a.u.

C	2.381511	2.390179	-0.193552
N	2.636354	1.034142	-0.097252
C	1.450356	0.357554	-0.012954
C	0.415285	1.278110	-0.045979
C	1.012262	2.578314	-0.155110
C	-0.967988	0.823331	0.000999
C	-1.261193	-0.558733	-0.082654
C	1.291693	-1.121666	0.165162
C	-0.141469	-1.552052	-0.264077
N	-2.513156	-1.036360	-0.064956
C	-2.093526	1.665809	0.094798
N	-3.345008	1.201832	0.124209
O	-0.300559	-2.680756	-0.694823

N	1.322292	-1.455687	1.586648
O	2.259931	-1.797447	-0.624333
H	3.187633	3.104532	-0.292808
H	0.508553	3.534461	-0.216701
H	-1.972014	2.747274	0.151531
H	2.166990	-1.102579	2.031604
H	1.271950	-2.465505	1.718158
H	1.848062	-2.635660	-0.904823
C	-3.490224	-0.133837	0.049225
H	3.539886	0.589306	-0.191643
H	-4.509661	-0.515759	0.082241

15 (B3LYP/D95++(d,p)) E= -739.43376 a.u.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.377959
C	1.371329	0.000000	1.788103
C	2.166020	0.003471	0.637125
N	1.318423	0.003145	-0.438705
C	3.618874	0.007151	0.623427
C	4.285714	0.005634	1.871346
C	1.970325	0.032828	3.107373
C	3.524107	0.027845	3.201443
N	5.616095	-0.035392	1.981398
C	4.406411	-0.004253	-0.540299
C	5.795765	-0.024250	-0.421755
N	3.878168	-1.165705	3.932633
H	3.948019	-0.001040	-1.527928
H	6.436557	-0.031704	-1.299406
O	1.342064	0.102775	4.164902
O	3.889002	1.266817	3.833418
H	3.372972	-1.202595	4.816584
H	4.883619	-1.182218	4.095353
H	3.269608	1.382046	4.574447
C	6.353312	-0.047591	0.863848
H	7.434311	-0.079520	0.998030
H	-0.818041	-0.003148	-0.708118
H	-0.865204	-0.000268	2.027158
H	1.601541	0.006594	-1.408472

16	(B3LYP/D95++(d,p))		E= -739.42254 a.u.
C	2.294471	2.477842	-0.174924
C	2.703080	1.152174	-0.106251
C	1.524130	0.363759	-0.025696
C	0.432190	1.219879	-0.044390
N	0.919282	2.511356	-0.130491
C	-0.953022	0.797305	0.001290
C	-1.230717	-0.595832	-0.075373
C	1.346793	-1.120170	0.135828
C	-0.097349	-1.572074	-0.233945
N	-2.469484	-1.107314	-0.062538
C	-2.056885	1.666855	0.091634
C	-3.342313	1.131904	0.114045
O	-0.256960	-2.725664	-0.601793
N	1.439220	-1.464003	1.555706
O	2.274842	-1.800903	-0.695555
H	2.873275	3.388016	-0.261962
H	0.359666	3.348551	-0.201732
H	-1.915798	2.744550	0.153175
H	-4.215112	1.775883	0.189320
H	2.317056	-1.124949	1.945078
H	1.393604	-2.475906	1.675302
H	1.861238	-2.656798	-0.911373
C	-3.499049	-0.263870	0.039219
H	-4.492815	-0.710465	0.060604
H	3.724720	0.796749	-0.136980

Transition States

6MIQ-TS	(B3LYP/D95++(d,p))		E= -648.30581 a.u.
C	0.000000	0.000000	0.000000
N	0.000000	0.000000	1.365046
C	1.301757	0.000000	1.807692
C	2.154287	-0.016476	0.692922
C	1.316694	-0.017522	-0.468585
C	3.615366	-0.063139	0.887389
C	4.101270	-0.032767	2.149802

C	1.731659	-0.064341	3.178500
C	3.248622	0.203505	3.377646
N	3.697517	-0.654032	4.594623
O	0.992879	-0.299816	4.141897
O	3.492938	1.420472	3.968855
C	1.685822	-0.029440	-1.929412
C	4.538986	-0.107023	-0.306460
H	-0.924408	0.014252	-0.563981
H	-0.803873	0.009542	1.979049
H	5.177031	0.016923	2.318730
H	2.879322	-1.042317	5.076861
H	4.428012	-1.352022	4.441719
H	2.259702	-0.923194	-2.202271
H	2.287233	0.844221	-2.207438
H	0.782102	-0.017161	-2.548401
H	4.413288	0.781265	-0.938511
H	5.584060	-0.146583	0.015466
H	4.341864	-0.983108	-0.936854
H	3.927075	0.468038	4.912837

7MIQ-TS (B3LYP/D95++(d,p)) E= -648.30196 a.u.

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.392509
C	1.273725	0.000000	2.110522
C	2.450132	0.002061	1.409300
C	2.523047	0.096470	-0.045376
C	1.201703	-0.020024	-0.890646
N	-1.285989	-0.136264	-0.434809
C	-2.130481	-0.211389	0.657255
C	-1.378916	-0.121050	1.816564
O	3.573445	0.325796	-0.648203
N	1.259669	1.212332	-1.882131
O	1.172860	-0.966145	-1.871640
C	1.293764	-0.023203	3.616900
C	-1.958554	-0.161801	3.205633
H	3.406644	0.009544	1.927078
H	-1.529260	-0.350835	-1.393619
H	-3.200092	-0.319541	0.533033

H	0.531409	1.925979	-1.814028
H	2.200474	1.618722	-1.897434
H	2.318716	-0.003043	3.996913
H	0.801637	-0.926437	3.998611
H	0.750326	0.835056	4.031233
H	-1.715596	0.740004	3.781324
H	-1.594643	-1.023634	3.778597
H	-3.050199	-0.237590	3.157186
H	1.173811	0.241912	-2.571073

6IIQ-TS (B3LYP/D95 (d,p)) E= -1010.95972 a.u.

H	2.633893	0.958366	-3.777163
C	2.740994	0.432275	2.511168
N	3.575080	0.618799	1.444727
C	2.839382	0.536518	0.285470
C	1.501798	0.276636	0.626560
C	1.438339	0.206228	2.054363
C	0.503458	0.065645	-0.437852
C	0.897185	0.143119	-1.733155
C	3.359258	0.537101	-1.055460
C	2.270506	0.621370	-2.156458
N	2.825415	-0.144997	-3.390466
O	4.559807	0.485274	-1.351968
O	2.221787	1.850657	-2.760397
C	0.258656	-0.072632	2.947197
C	-0.919473	-0.176373	-0.103050
C	-1.684957	-1.325020	-0.186338
C	-3.008150	-0.972228	0.277679
C	-2.985867	0.409752	0.623885
N	-1.699183	0.864493	0.402993
C	-4.207664	-1.697779	0.430362
C	-5.341846	-1.036322	0.905473
C	-5.300017	0.340435	1.232095
C	-4.122958	1.082109	1.096376
C	-1.239635	-2.688647	-0.632507
H	3.108805	0.466229	3.528792
H	4.571979	0.787244	1.467243
H	0.156254	0.070377	-2.527570

H	3.822515	-0.343172	-3.247976
H	2.307680	-0.957673	-3.729975
H	-0.480498	0.735201	2.910561
H	0.583680	-0.186444	3.986793
H	-0.259874	-0.990371	2.649794
H	-1.402842	1.829983	0.421895
H	-4.251581	-2.755641	0.178102
H	-6.275552	-1.581829	1.026772
H	-6.200545	0.830360	1.596925
H	-4.094465	2.140110	1.350069
H	-1.810088	-3.028357	-1.507163
H	-0.179095	-2.686868	-0.902278
H	-1.386279	-3.436146	0.158473

7IIQ-TS (B3LYP/D95 (d,p)) E= -1010.95444 a.u.

H	-1.868712	0.085570	-4.866336
C	-1.894772	0.047098	-2.038002
C	-1.341006	0.085398	-0.758672
C	0.118148	0.105574	-0.618164
C	0.914125	0.193789	-1.734447
C	0.378048	0.307084	-3.086177
C	-1.141853	0.005607	-3.332508
N	-3.251616	-0.042135	-1.920526
C	-3.596733	-0.026644	-0.580316
C	-2.444816	0.071004	0.182363
O	1.068529	0.636812	-4.054732
N	-1.604338	1.120625	-4.350357
O	-1.435799	-1.042747	-4.148085
C	0.762112	-0.017508	0.699905
C	-2.442373	0.203563	1.683751
C	1.740647	0.761077	1.303344
C	2.022722	0.145905	2.577693
C	1.201321	-1.013157	2.687993
N	0.426955	-1.075072	1.547258
C	2.901431	0.468098	3.633949
C	2.951261	-0.369340	4.748411
C	2.135934	-1.525143	4.830312
C	1.251467	-1.863834	3.803447

C	2.362787	2.028914	0.790190
H	1.996333	0.194797	-1.644430
H	-3.868368	-0.267538	-2.689787
H	-4.631146	-0.061728	-0.265683
H	-2.283150	1.824437	-4.053282
H	-0.768336	1.539907	-4.773347
H	-1.756282	0.989866	2.016140
H	-2.137292	-0.718813	2.189916
H	-3.446830	0.458841	2.037940
H	-0.147721	-1.857389	1.268836
H	3.536434	1.349988	3.577336
H	3.626714	-0.138381	5.569529
H	2.198875	-2.160589	5.711347
H	0.625110	-2.751093	3.872261
H	3.432248	1.891429	0.582515
H	2.277681	2.834667	1.530601
H	1.884907	2.364671	-0.134087

1TS	(B3LYP/D95++(d,p))		E= -608.98056 a.u.
H	0.000000	0.000000	0.000000
C	0.000000	0.000000	6.325790
C	0.961474	0.000000	5.336384
C	0.276515	-0.191850	4.095106
C	-1.090939	-0.319479	4.372950
N	-1.239539	-0.201897	5.729928
C	-2.140930	-0.569618	3.390816
C	-1.764727	-0.617083	2.092244
C	0.743616	-0.358022	2.732106
C	-0.365660	-0.256589	1.636958
N	0.114886	-1.102597	0.436053
O	1.911259	-0.558130	2.392962
O	-0.339809	0.952985	0.977906
H	0.086037	0.128289	7.396623
C	-3.570578	-0.716814	3.850382
H	-2.511722	-0.716670	1.304867
H	1.097416	-1.366241	0.582193
H	-0.463508	-1.890753	0.139132
H	-3.924692	0.198682	4.345319

H	-4.233903	-0.912646	3.003169
H	-3.681733	-1.545089	4.564271
H	2.026878	0.131763	5.471361
H	-2.118876	-0.254249	6.225416

2TS (B3LYP/D95++(d,p)) E= -608.97858 a.u.

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.848018
C	0.746967	0.000000	4.022799
C	2.162617	0.296757	4.110827
C	2.809569	0.694735	2.974318
C	2.087354	0.904365	1.716849
C	0.697430	0.211776	1.530299
C	-1.321433	-0.404699	3.177052
C	-1.351237	-0.620581	4.550623
N	-0.094767	-0.382762	5.053556
O	2.540385	1.589270	0.796805
N	-0.101479	1.066850	0.520401
O	0.790579	-0.904502	0.734109
C	2.868081	0.175168	5.437163
H	3.859564	0.976779	2.988596
H	-2.165294	-0.925207	5.195329
H	-0.988800	1.467586	0.829263
H	0.523747	1.766015	0.101040
H	3.924647	0.440022	5.347156
H	2.805469	-0.853018	5.819288
H	2.414942	0.836131	6.189118
H	0.167891	-0.468092	6.025054
H	-2.154659	-0.554612	2.501428

3TS (B3LYP/D95++(d,p)) E= -625.03475 a.u.

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	6.250817
N	0.937381	0.000000	5.262608
C	0.252479	-0.130849	4.068935
C	-1.093066	-0.224503	4.419917
N	-1.236613	-0.141466	5.783013
C	-2.154241	-0.423238	3.427049

C	-1.781188	-0.471873	2.127953
C	0.746807	-0.297043	2.726891
C	-0.370880	-0.182971	1.646197
N	0.054633	-1.095248	0.466222
O	1.922077	-0.503512	2.414243
O	-0.283940	0.998820	0.949313
H	0.260055	0.109765	7.296841
C	-3.579043	-0.522586	3.902833
H	-2.533811	-0.535128	1.342038
H	1.017667	-1.425171	0.594947
H	-0.581147	-1.847697	0.194472
H	-3.875305	0.397095	4.422626
H	-4.262814	-0.688931	3.064851
H	-3.692162	-1.340009	4.625342
H	1.941144	0.090430	5.359212

4TS	(B3LYP/D95++(d,p))		E= -625.03232 a.u.
H	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.843070
C	0.605294	0.000000	4.084993
C	2.056268	0.004597	4.241570
C	2.831226	0.025372	3.115907
C	2.270889	0.141845	1.768395
C	0.722731	-0.067598	1.535266
N	-1.342229	-0.165949	3.090800
C	-1.491467	-0.237504	4.457653
N	-0.338691	-0.135770	5.089100
O	2.954154	0.440452	0.787820
N	0.308019	1.036628	0.507707
O	0.374810	-1.124302	0.744035
C	2.628376	-0.033292	5.628735
H	3.916701	0.045973	3.179071
H	-2.460923	-0.353258	4.926626
H	-0.352450	1.760772	0.797837
H	1.152037	1.431675	0.076534
H	3.721530	-0.041775	5.611143
H	2.266262	-0.921951	6.160325
H	2.280513	0.831361	6.207692

H	-2.051687	-0.356242	2.393932

5TS	(B3LYP/D95++(d,p))	E= -647.08591 a.u.

H	3.395162	-0.356416	0.715376
C	-2.765278	-1.558989	0.147162
N	-1.460470	-1.827112	0.043902
C	-0.614238	-0.792823	-0.047656
C	-1.011190	0.569890	-0.053782
C	-0.014067	1.663133	-0.153640
C	1.305410	1.384578	-0.091336
C	0.839382	-1.109739	-0.227862
C	1.822342	0.000530	0.198970
N	3.181418	-0.302451	-0.458103
O	1.247852	-2.170058	-0.678303
O	2.245294	-0.167039	1.501370
H	-3.430622	-2.417528	0.237569
C	-0.505249	3.087698	-0.260449
H	2.035813	2.193687	-0.074147
H	3.149452	-1.220157	-0.918912
H	3.587786	0.418386	-1.056949
H	-1.079870	3.379497	0.628907
H	0.337345	3.778664	-0.353948
H	-1.158025	3.226819	-1.132228
C	-2.393828	0.818116	0.027356
C	-3.280486	-0.253599	0.135751
H	-2.772995	1.835849	0.013261
H	-4.352643	-0.087859	0.208849

6TS	(B3LYP/D95++(d,p))	E= -647.10020 a.u.

H	2.081273	-1.938702	0.919276
C	-0.316815	-0.704396	-0.015677
C	-1.004211	0.532980	0.007450
C	-0.244243	1.804685	0.041373
C	1.107071	1.806658	-0.108030
C	1.863177	0.561281	-0.310127
C	1.180298	-0.700235	0.236795
N	-0.914137	-1.889854	-0.157288
C	-2.255060	-1.916784	-0.234680

O	2.984613	0.516517	-0.811558
N	1.868033	-1.948571	-0.266550
O	1.501236	-0.851587	1.577326
C	-1.002890	3.099550	0.184525
H	1.668777	2.736581	-0.162720
H	-2.712788	-2.897704	-0.357604
H	1.207899	-2.646968	-0.618908
H	2.649406	-1.741736	-0.895906
H	-0.317000	3.949887	0.215950
H	-1.598182	3.102747	1.106960
H	-1.697408	3.252392	-0.652119
C	-2.405368	0.477013	-0.050944
C	-3.042426	-0.763794	-0.163731
H	-2.997596	1.387668	-0.023158
H	-4.125639	-0.836374	-0.212774

7TS (B3LYP/D95++(d,p)) E= -647.09542 a.u.

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	6.452929
C	0.616843	0.000000	5.201224
C	-0.125451	-0.402592	4.086205
C	-1.469166	-0.821921	4.261282
C	-2.282672	-1.277915	3.106326
C	-1.786311	-1.174996	1.854686
C	0.495885	-0.480384	2.744602
C	-0.476664	-0.497089	1.548930
N	0.265808	-1.111014	0.343666
O	1.710886	-0.508572	2.568037
O	-0.622139	0.761925	1.005468
H	0.527259	0.316068	7.349022
C	-3.673709	-1.787082	3.383186
H	-2.411751	-1.423689	0.996910
H	1.258914	-1.243497	0.566854
H	-0.146768	-1.936752	-0.094201
H	-4.283234	-1.007228	3.854232
H	-4.159395	-2.106575	2.455904
H	-3.651994	-2.627392	4.086553
N	-2.051979	-0.839274	5.475394

C	-1.333485	-0.429473	6.528640
H	-1.847845	-0.445942	7.490080
H	1.651640	0.305678	5.066779

8TS (B3LYP/D95++(d,p)) E= -647.09571 a.u.

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.840446
C	0.736217	0.000000	4.046198
C	2.183738	0.332844	4.054237
C	2.800203	0.764742	2.921807
C	2.058553	0.992288	1.683745
C	0.705711	0.256115	1.519066
C	-1.340965	-0.391367	2.889365
C	-1.918521	-0.707902	4.120679
O	2.471226	1.713500	0.774472
N	-0.127193	1.074784	0.508485
O	0.822460	-0.866987	0.735115
C	2.927707	0.199356	5.353012
H	3.848263	1.056087	2.922924
H	-2.961702	-1.003565	4.197644
H	-1.018190	1.473657	0.808875
H	0.487913	1.776946	0.076848
H	3.983111	0.455579	5.225832
H	2.844496	-0.824262	5.736453
H	2.484626	0.845594	6.119382
N	0.185224	-0.327358	5.232979
C	-1.108983	-0.656135	5.264488
H	-1.520598	-0.901997	6.243419
H	-1.923845	-0.472746	1.973615

9TS (B3LYP/D95++(d,p)) E= -663.12813 a.u.

H	0.000000	0.000000	0.000000
C	0.000000	0.000000	6.276788
N	0.597412	0.000000	5.080435
C	-0.122865	-0.480852	4.061678
C	-1.439161	-0.974296	4.209902
C	-2.216687	-1.486963	3.059266
C	-1.723219	-1.357572	1.808969

C	0.524065	-0.578683	2.707774
C	-0.453614	-0.598938	1.516586
N	0.311346	-1.118690	0.288026
O	1.732036	-0.640807	2.547563
O	-0.669805	0.674837	1.033105
H	0.572010	0.408198	7.109171
C	-3.579008	-2.087878	3.312206
H	-2.326615	-1.651172	0.949959
H	1.307582	-1.234624	0.508950
H	-0.073080	-1.932102	-0.195811
H	-4.263701	-1.350143	3.751402
H	-4.023096	-2.441423	2.377438
H	-3.524093	-2.936407	4.006581
C	-1.931918	-0.944068	5.528831
N	-1.229525	-0.458740	6.559166
H	-2.926796	-1.318805	5.762141

10TS	(B3LYP/D95++(d,p))		E= -663.14419 a.u.
H	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.845281
C	0.875121	0.000000	3.953520
C	2.186897	0.679878	3.878920
C	2.499824	1.439818	2.795724
C	1.561527	1.618651	1.676144
C	0.521748	0.498192	1.512538
N	-1.234795	-0.504041	2.900628
C	-1.599001	-1.065022	4.065277
O	1.623457	2.547901	0.875021
N	-0.572678	0.907083	0.555144
O	1.052894	-0.527240	0.747594
C	3.133619	0.561413	5.045307
H	3.425830	2.008850	2.753393
H	-2.609553	-1.468722	4.116761
H	-1.514749	0.723886	0.910079
H	-0.435769	1.853026	0.185521
H	4.063540	1.100294	4.847111
H	3.379361	-0.490245	5.242540
H	2.690485	0.969005	5.963451

C	0.380919	-0.639233	5.099795
N	-0.847600	-1.178721	5.164406
H	0.981531	-0.716200	6.004514

11TS (B3LYP/D95++(d,p)) E= -739.38288 a.u.

H	-0.875504	2.900345	0.844602
C	3.079888	-1.741671	0.042749
N	2.993606	-0.385073	-0.114824
C	1.670842	-0.008223	-0.078861
C	0.890806	-1.159544	0.084910
C	-0.571840	-1.081637	0.043519
C	-1.170724	0.201350	-0.015336
C	1.136787	1.326122	-0.269169
C	-0.314636	1.444164	0.233596
N	-0.962493	2.696951	-0.329776
O	1.771020	2.294612	-0.696398
O	-0.299805	1.832505	1.557240
H	4.035972	-2.248053	0.066828
C	-1.424793	-2.192062	-0.011652
N	-2.481222	0.399059	-0.187090
H	-0.341789	3.221874	-0.951461
H	-1.898570	2.511717	-0.701459
C	1.790759	-2.259692	0.160328
H	1.549465	-3.307501	0.284423
H	3.760276	0.267441	-0.212349
C	-2.803733	-1.988928	-0.146051
C	-3.282017	-0.677895	-0.251010
H	-1.018452	-3.200343	0.032322
H	-4.344376	-0.483412	-0.394918
H	-3.494016	-2.827456	-0.191029

12TS (B3LYP/D95++(d,p)) E= -739.36127 a.u.

H	-2.749869	-2.000197	0.223780
C	-1.401520	0.480594	-0.023834
C	-0.293224	1.309311	-0.126358
C	1.061874	0.767922	-0.076355
C	1.255374	-0.634124	0.039465
C	0.073276	-1.562284	-0.043885

C	-1.377140	-1.001375	0.179577
N	-2.521897	1.271018	0.056693
C	-2.152027	2.600402	-0.004991
O	0.197290	-2.745996	-0.323148
N	-2.278212	-1.788654	-0.846132
O	-2.019833	-1.455437	1.290627
N	2.462275	-1.215078	0.142249
H	-2.888181	3.391700	0.038995
H	-2.736254	-1.273131	-1.600084
H	-1.756302	-2.601504	-1.192095
C	-0.775071	2.661256	-0.129563
H	-0.193525	3.571170	-0.203993
C	2.216065	1.573679	-0.099965
C	3.468120	0.971693	0.007587
H	2.126822	2.653584	-0.192297
C	3.539364	-0.428222	0.136923
H	4.504304	-0.925520	0.235717
H	-3.431957	0.926225	0.331573
H	4.379601	1.565025	-0.002696

13TS (B3LYP/D95++(d,p)) E= -755.42685 a.u.

H	-0.964525	2.878189	0.833932
C	3.105968	-1.684611	0.044310
N	2.992765	-0.329807	-0.108971
C	1.663005	0.020951	-0.075457
C	0.907303	-1.148195	0.083593
C	-0.554053	-1.089337	0.040230
C	-1.177302	0.178247	-0.017755
C	1.105483	1.346223	-0.260165
C	-0.354642	1.440695	0.228043
N	-1.021161	2.677439	-0.345578
O	1.723343	2.329894	-0.674796
O	-0.374715	1.824282	1.551514
H	4.072011	-2.171674	0.067949
C	-1.418983	-2.189805	-0.017200
N	-2.495089	0.318554	-0.189289
H	-0.396222	3.220216	-0.948034
H	-1.944334	2.484477	-0.743347

C	1.827625	-2.230291	0.157670
H	1.606442	-3.282933	0.277085
H	3.747164	0.337607	-0.203322
N	-2.749774	-2.062587	-0.149346
C	-3.216605	-0.813188	-0.247690
H	-1.032913	-3.207869	0.031942
H	-4.290617	-0.700755	-0.391129

14TS (B3LYP/D95++(d,p)) E= -755.40368 a.u.

H	-2.737318	-2.008549	0.237072
C	-1.392422	0.477280	-0.023752
C	-0.285859	1.309908	-0.129452
C	1.064125	0.763082	-0.078002
C	1.261849	-0.631892	0.042276
C	0.080167	-1.568094	-0.047202
C	-1.368312	-1.006476	0.179623
N	-2.512721	1.266837	0.057803
C	-2.145083	2.596820	-0.006796
O	0.217471	-2.746142	-0.334558
N	-2.276426	-1.792924	-0.838821
O	-1.999875	-1.461399	1.295798
N	2.480219	-1.182303	0.149565
H	-2.882659	3.386675	0.038016
H	-2.745478	-1.273861	-1.583666
H	-1.763301	-2.604839	-1.198774
C	-0.768640	2.661043	-0.133460
H	-0.187613	3.571031	-0.208778
C	2.243445	1.535781	-0.100221
N	3.461528	0.999423	0.005372
H	2.194530	2.619971	-0.199945
C	3.515636	-0.339469	0.136980
H	4.507373	-0.778039	0.238565
H	-3.423946	0.922816	0.330192

15TS (B3LYP/D95++(d,p)) E= -739.37825 a.u.

H	-0.957984	2.867408	0.901436
C	3.107233	-1.691305	0.059325
C	3.100122	-0.321189	-0.122758

C	1.732555	0.090093	-0.102483
C	0.942468	-1.052198	0.076500
C	-0.513566	-1.071675	0.032196
C	-1.164858	0.187837	-0.015316
C	1.098521	1.393554	-0.292421
C	-0.347931	1.451518	0.247235
N	-1.043941	2.693041	-0.277875
O	1.640717	2.392587	-0.763357
O	-0.336572	1.803664	1.581375
H	3.930372	-2.389596	0.129560
C	-1.316476	-2.219162	-0.035635
N	-2.481703	0.328317	-0.182388
H	-0.432999	3.248379	-0.884193
H	-1.973053	2.494092	-0.657848
N	1.793314	-2.123791	0.168634
C	-2.703147	-2.072533	-0.165502
C	-3.236320	-0.781835	-0.254994
H	-0.879082	-3.216010	-0.007041
H	-4.306380	-0.631752	-0.393847
H	-3.356583	-2.939401	-0.219189
H	1.513417	-3.084087	0.309134
H	3.963841	0.319369	-0.237653

16TS	(B3LYP/D95++(d,p))		E= -739.36139 a.u.
H	-2.572844	-2.078395	0.734650
C	-1.483835	0.459658	-0.016608
C	-0.342205	1.248444	-0.107889
C	1.020872	0.751081	-0.033056
C	1.218656	-0.656934	-0.058086
C	0.019215	-1.548022	-0.252953
C	-1.350691	-1.016905	0.249785
C	-2.611275	1.329288	-0.038846
C	-2.124285	2.624441	-0.161700
O	0.105136	-2.655347	-0.766620
N	-2.441859	-1.876628	-0.427365
O	-1.598071	-1.433453	1.531240
N	2.420894	-1.241526	0.007674
H	-2.648909	3.568081	-0.229992

H	-3.138040	-1.394358	-0.997382
H	-1.992991	-2.654312	-0.927221
N	-0.749063	2.567045	-0.190707
H	-0.140162	3.364652	-0.301182
C	2.169089	1.559174	0.059714
C	3.421568	0.949223	0.136289
H	2.091730	2.644804	0.085584
C	3.496429	-0.454215	0.113643
H	4.460817	-0.957232	0.180814
H	-3.656399	1.060763	0.052565

Appendix 2

(Natural population analysis at the B3LYP/D95(d,p) for OBQ, MIQ and IIQ)

OBQ	MIQ	IIQ
C 0.47775	C 0.49445	C 0.48597
C -0.26305	C -0.31578	C -0.28811
C -0.17949	C 0.46915	C 0.46848
C -0.17949	O -0.52332	O -0.52268
C -0.26305	C 0.06344	C -0.01088
C 0.47775	C 0.08615	C 0.08610
O -0.49668	H 0.22563	H 0.23340
H 0.23386	O -0.54984	O -0.55072
H 0.22761	C -0.10677	C -0.10137
H 0.22761	N -0.53944	C 0.16739
H 0.23386	C -0.64174	N -0.53756
O -0.49668	C -0.05806	C -0.05728
	C 0.02064	C 0.02119
	H 0.44525	H 0.44591
	H 0.22871	C -0.03730
	H 0.22871	N -0.60273
	H 0.22874	C -0.64515
	H 0.21357	H 0.21430
	C -0.64515	C -0.64803
	H 0.22558	H 0.42652
	H 0.22503	C -0.08830
	H 0.22503	C 0.20048
		C -0.25108
		C -0.20057
		H 0.22196
		H 0.22449
		H 0.23685
		H 0.22994
		H 0.22453
		H 0.22815
		H 0.21482
		C -0.20800
		C -0.23035
		H 0.21631
		H 0.21682
		H 0.21651

(END)