Supplementary information
for

Air Oxidized Active Carbon as a Green Heterogeneous Catalyst for Catalytic Aerobic Oxidative Aromatizations of N-Heterocycles

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S1 Computational details

All density functional theory level computations were carried out with TURBOMOLE 7.4[1] and ORCA 4.1[2] program packages. Transitions states were searched for using ORCA, whereas the geometries, vibrational frequencies, and final single-point energies were computed with TURBOMOLE. Lowest energy conformers were searched with CREST[3] and GFN-xTB.[4] Structures were optimised using a dispersion corrected hybrid functional PBE0-D3BJ[5, 6] using def2-TZVP basis sets[7] and final single-point energies were calculated using resolution-of-identity random phase approximation (RI-RPA).[8, 9] Orbitals for the RI-RPA calculations were computed on PBE0-D3BJ/def2-QZVPP level of theory in gas-phase and the core orbitals were kept frozen for computation of correlation energy. The (multipole accelerated) resolution-of-identity approximation for Coulomb term[10, 11] with corresponding auxiliary basis sets[12, 13] was used with TURBOMOLE. Additionally, the *m4* grid and default convergence criteria of 10^{-6} and 10^{-6} were used for density and energy, respectively. For RI-RPA calculations the *m5* grid and convergence threshold of 10^{-7} for energy was used. The 3D images were created using CYLview.[14]

In structure optimisations the solvation effects were accounted for using COSMO[15] with dielectric constant for toluene (2.38), whereas for final single-point energies the COSMO-RS solvation model was used as implemented in COSMOtherm19 program package[16-19] with BP_TZVPD_FINE_19.ctd parameter file based on BP86[20, 21]/def2-TZVPD computational level. The Gibbs free energies in solution were calculated according to published protocol: $G = E_{gas}(SCF) + \text{chem.pot.} + G_{solv}$,[22] where $E_{gas}(SCF)$ is the final single-point energy of the system in gas-phase, chem.pot. is the chemical potential calculated at the optimisation level using qRRHO approximation by Grimme,[23] and G_{solv} is the solvation free energy of each species in toluene from COSMO-RS. All thermodynamic functions were calculated at 298.15 K and vibrational frequencies were used without scaling. The reference state for the Gibbs free energies is 1 bar of ideal gas and 1 mol of liquid solvent.[22]

The 1-electron oxidation potentials for THQs **1e–l** were calculated from Eq. 1:

$$E^\circ = -\frac{\Delta G}{nF} - E^\circ_{ref} \qquad \text{Eq. 1}$$

Where ΔG is the reaction free energy between the reduced and oxidised forms in acetonitrile, n is the amount of transferred electron, F is the Faraday's constant, and E°_{ref} is the absolute potential of SCE (4.422 V)[24] in acetonitrile.

S2 Oxidation potentials for 6-R-THQs

Table S1. Computed one-electron oxidation potentials for 6-R-THQs (**1e–l**).

Entry	Substrate	R	$E_{ox}°$ (V)[a]
1	**1f**	OMe	0.75
2	**1g**	Me	0.97
3	**1e**	H	1.09
4	**1h**	F	1.08
5	**1i**	Cl	1.18
6	**1j**	Br	1.29
7	**1k**	COOMe	1.38
8	**1l**	CN	1.52

a Referenced to SCE in acetonitrile

S3 Reaction free energies

Ortho-benzoquinone (*o*BQ) and phenanthrenequinone (PQ) were chosen as the model quinoidic fragments for comparison of the activation free energy barriers with substrate **1e**.[25]

Computed activation free energy barriers for bimolecular hydride abstraction[26] in Figure S1 for **TS1** from C4 was 1.8 kcal/mol and 3.4 kcal/mol higher than from C2 with *o*-BQ and PQ, respectively, and supported the experimental observation that deuteriums at C4-position did not affect the reaction rate, see Fig. S1. The activation free energy barriers for bimolecular hydride abstraction from 2C were 27.1 kcal/mol and 31.3 kcal/mol with *o*-BQ and PQ, respectively, which supported the experimentally observed spoor reactivity of PQ with **1e**.

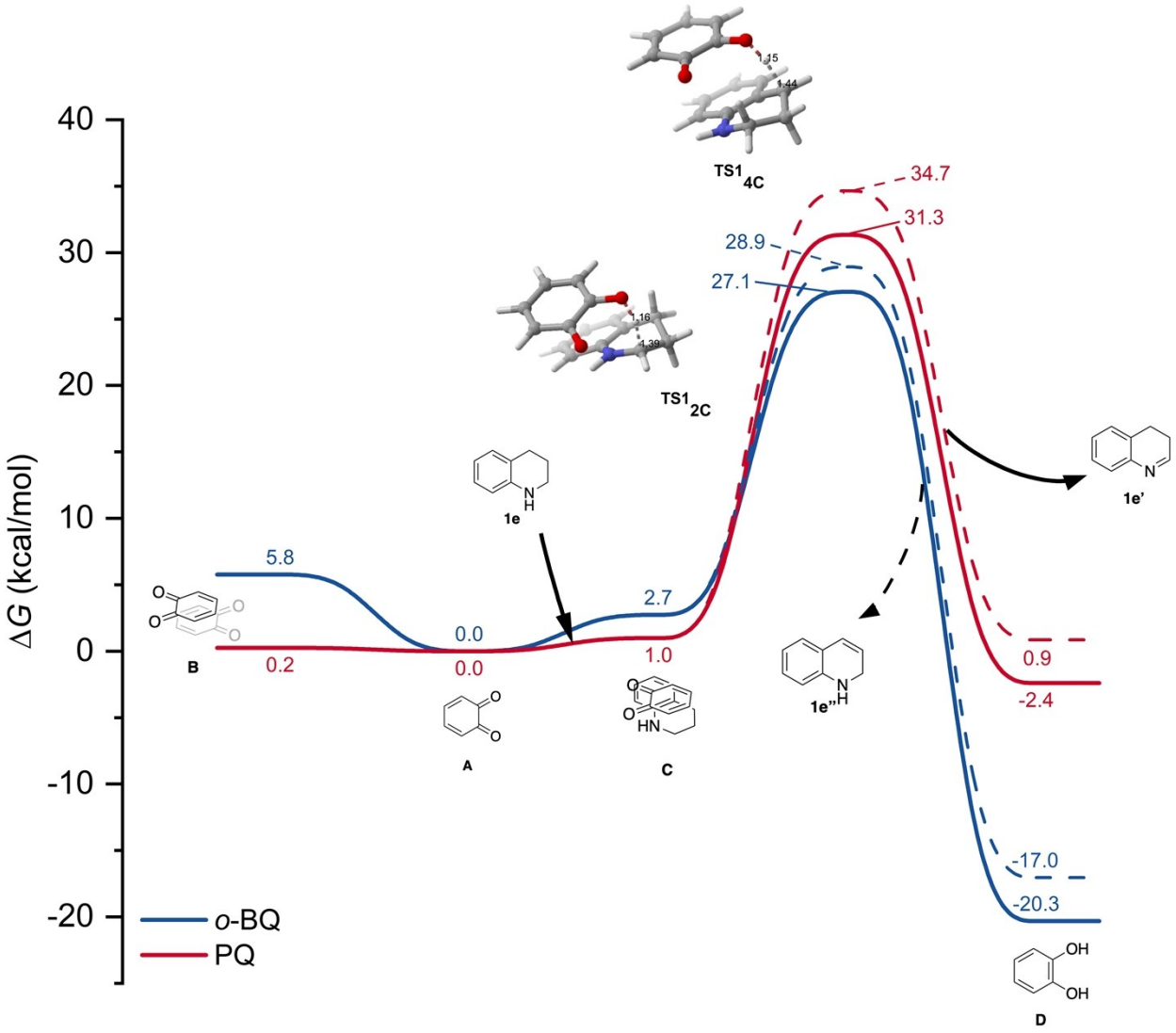

Fig. S1 The activation free energy barriers for direct bimolecular hydride abstraction from C2 (full lines) and C4 (dashed lines) for *o*-BQ (blue) and PQ (red). The structures are depicted with *o*-BQ for clarity and structures with PQ are similar.

Next, we investigated the reaction free energies for the hemiaminal pathway with **1e**. The formation of the hemiaminal proceeds through a zwitterionic species and for similar imine formation reactions, the reaction free energy barrier for the C-N bond formation has been shown to be unfeasible without a mediator molecule.[27,28] Since hydroxyl groups are abundantly present in the carbon materials used in this work, we used catechol with *o*-BQ and phenanthrenediol with PQ to stabilize the charged species and to mediate the proton transfer. The employed active carbon catalysts are, in essence, amorphous on contrary to, *e.g.*, highly ordered 2D graphitic surfaces, and thus the surface of the catalyst is uneven, non-uniform and has abundant pores present. Concurrently, the quinone-hydroquinone orientations presented in **TS2**, **E**, and **TS3** in Fig. S2 are plausible.

With *o*-BQ the activation free energy barrier for the hemiaminal formation is the proton transfer in **TS3**: 21.2 kcal/mol, whereas for PQ it is either the C-N bond formation in **TS2** (21.3 kcal/mol) or proton transfer in **TS3** (21.8 kcal/mol). With both model quinones the formation of the hemiaminal (**F**) was endergonic by 2.9 and 1.0 kcal/mol for *o*-BQ and PQ, respectively. The highest energy transition state for both model quinones was the hydride abstraction in **TS5** with activation free energy barrier of 35.4 (PQ) and 28.5 (*o*-BQ) kcal/mol. The activation free energy barrier with PQ also supports the poor reactivity with **1e**.

Structures **TS4** and **G** were not located for PQ and a DRC calculation connected the PQ's **TS5** to intermediates **F** and **D**. With *o*-BQ, the DRC calculations from both **TS4** and **TS5** connected to intermediate **G**, which was a minimum on optimization level of theory (PBE0-D3BJ/def2-TZVP).

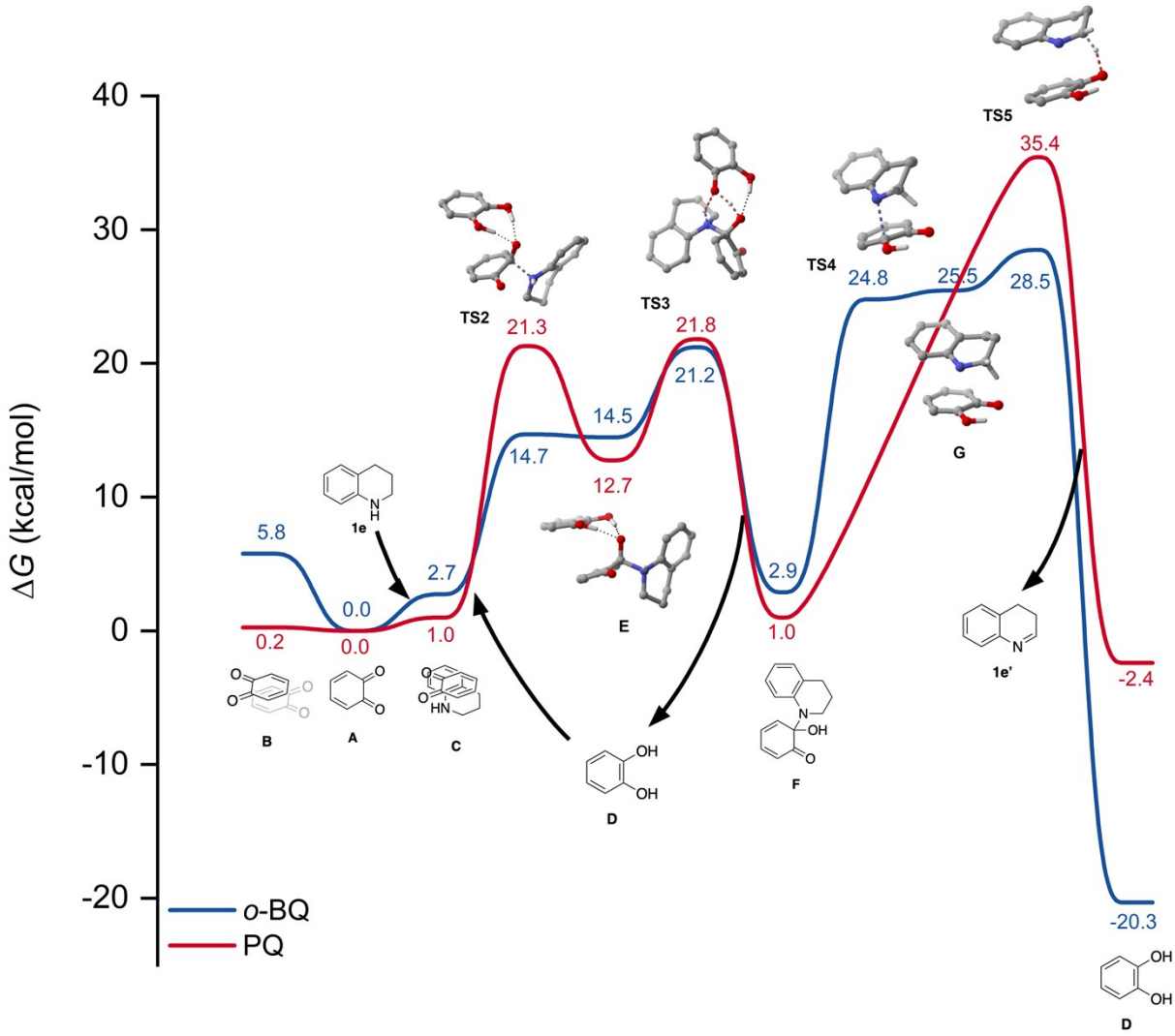

Fig. S2. Activation free energy barriers for the hemiaminal pathway with *o*-BQ (blue line) and PQ (red line). The structures are depicted with *o*-BQ for clarity and structures with PQ are similar. Structures **TS4** and **G** were not located for PQ and a DRC calculation connected the PQ's **TS5** to intermediates **F** and **D**.

S4 NBO charges

The NBO-charges in Table S1 were computed on PBE0-D3BJ/def2-QZVPP//PBE0-D3BJ/def2-TZVP level of theory in gas-phase. The NBO charge located on the free THQ's nitrogen correlated well (R^2 = 0.9523) with the measured reaction rates. For the hemiaminal structures, we found no or poor correlation between the NBO charges and reaction rates.

Table S2. Computed NBO charges.

			THQ NBO			**PQ-hemiaminal NBO**			***o*-BQ-hemiaminal NBO**			
Entry	Substrate	6-R	N(1)	C(2)	H(2, ax)	N(1)	C(2)	H(2, ax)	N(1)	C(2)	H(2, ax)	$\log(k_X/k_H)$
1	**1f**	OMe	-0.6249	-0.2183	0.1803	-0.4764	-0.2218	0.2120	-0.4517	-0.2157	0.1915	0.13
2	**1g**	Me	-0.6210	-0.2178	0.1818	-0.4856	-0.1987	0.2071	-0.4519	-0.2147	0.1923	0.09
3	**1e**	H	-0.6187	-0.2177	0.1831	-0.4834	-0.1988	0.2066	-0.4525	-0.2145	0.1929	0.00
4	**1h**	F	-0.6214	-0.2186	0.1828	-0.4774	-0.2223	0.2127	-0.4532	-0.2154	0.1929	0.08
5	**1i**	Cl	-0.6163	-0.2183	0.1848	-0.4766	-0.2227	0.2130	-0.4517	-0.2149	0.1939	0.05
6	**1j**	Br	-0.6154	-0.2182	0.1853	-0.4767	-0.2228	0.2131	-0.4517	-0.2148	0.1942	0.02
7	**1k**	COOMe	-0.6018	-0.2173	0.1893	-0.4683	-0.2001	0.2058	-0.4468	-0.2139	0.1958	-0.19
8	**1l**	CN	-0.5989	-0.2178	0.1918	-0.4653	-0.2008	0.2071	-0.4463	-0.2142	0.1972	-0.29
9	-	**R^2**	**0.9523**	0.4219	0.9329	0.6484	0.3123	0.3629	0.8610	0.6666	0.9017	-

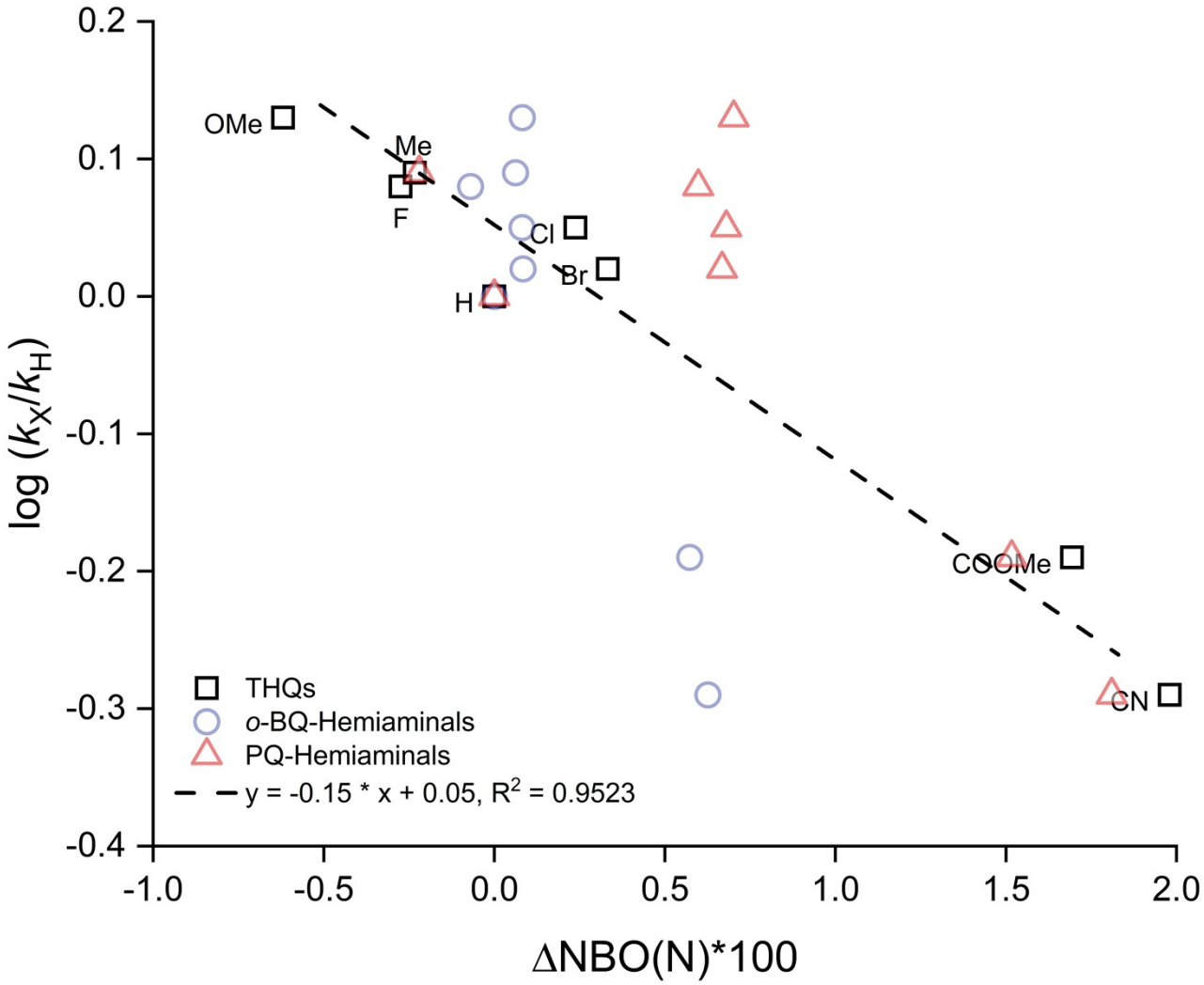

Figure S3. The $\log(k_X/k_H)$ values *versus* ΔNBO(N) charges.

References

1. F. Furche, R. Ahlrichs, C. Hättig, W. Klopper, M. Sierka and F. Weigend, *WIREs Computational Molecular Science*, 2014, **4**, 91-100.
2. F. Neese, *WIREs Computational Molecular Science*, 2018, **8**, e1327.
3. P. Pracht, F. Bohle and S. Grimme, *Physical Chemistry Chemical Physics*, 2020, **22**, 7169-7192.
4. S. Grimme, C. Bannwarth and P. Shushkov, *Journal of Chemical Theory and Computation*, 2017, **13**, 1989-2009.
5. C. Adamo and V. Barone, *The Journal of Chemical Physics*, 1999, **110**, 6158-6170.
6. S. Grimme, S. Ehrlich and L. Goerigk, *Journal of Computational Chemistry*, 2011, **32**, 1456-1465.
7. F. Weigend and R. Ahlrichs, *Physical Chemistry Chemical Physics*, 2005, **7**, 3297-3305.
8. H. Eshuis, J. E. Bates and F. Furche, *Theoretical Chemistry Accounts*, 2012, **131**, 1084.
9. H. Eshuis, J. Yarkony and F. Furche, *The Journal of Chemical Physics*, 2010, **132**, 234114.
10. K. Eichkorn, O. Treutler, H. Öhm, M. Häser and R. Ahlrichs, *Chemical Physics Letters*, 1995, **240**, 283-290.
11. M. Sierka, A. Hogekamp and R. Ahlrichs, *The Journal of Chemical Physics*, 2003, **118**, 9136-9148.
12. F. Weigend, *Physical Chemistry Chemical Physics*, 2006, **8**, 1057-1065.
13. F. Weigend, M. Häser, H. Patzelt and R. Ahlrichs, *Chemical Physics Letters*, 1998, **294**, 143-152.
14. C. Y. Legault, *CYLview20*, 2.0, **2020**.
15. A. Schäfer, A. Klamt, D. Sattel, J. C. W. Lohrenz and F. Eckert, *Physical Chemistry Chemical Physics*, 2000, **2**, 2187-2193.
16. A. Klamt, *COSMOtherm*, 19, COSMOlogic GmbH & Co. KG, a Dassault Systèmes company.: **2019**.
17. F. Eckert and A. Klamt, *AIChE Journal*, 2002, **48**, 369-385.
18. A. Klamt, V. Jonas, T. Bürger and J. C. W. Lohrenz, *The Journal of Physical Chemistry A*, 1998, **102**, 5074-5085.
19. A. Klamt, *The Journal of Physical Chemistry*, 1995, **99**, 2224-2235.
20. A. D. Becke, *Physical Review A*, 1988, **38**, 3098-3100.
21. J. P. Perdew, *Physical Review B*, 1986, **33**, 8822-8824.
22. A. Hellweg and F. Eckert, *AIChE Journal*, 2017, **63**, 3944-3954.
23. S. Grimme, *Chemistry – A European Journal*, 2012, **18**, 9955-9964.
24. H. G. Roth, N. A. Romero and D. A. Nicewicz, *Synlett*, 2016, **27**, 714-723.
25. T. Wirtanen, S. Aikonen, M. Muuronen, M. Melchionna, M. Kemell, F. Davodi, T. Kallio, T. Hu and J. Helaja, *Chemistry – A European Journal*, 2019, **25**, 12288-12293.
26. C. A. Morales-Rivera, P. E. Floreancig and P. Liu, *J. Am. Chem. Soc.*, 2017, **139**, 17935-17944.
27. P. J. Silva, *PeerJ Organic Chemistry*, 2020, **2**, e4.
28. R. Pérez-Soto, M. Besora and F. Maseras, *Org. Lett.*, 2020, **22**, 2873-2877.

XYZ parameters

E(PBE0): The SCF energy in Hartrees at the optimisation level of theory (PBE0-D3BJ/def2-TZVP in COSMO)
chem.pot.: chemical potential in Hartrees calculated as explained in the methods section.
E(RPA): The gas-phase single-point energy calculated with random phase approximation based on PBE0 orbitals
Gsolv: The COSMO-RS solvation free energy of each species in toluene in kcal/mol
i-freq.: The imaginary frequency for a transition state in cm-1

1e
21
E(PBE0)=-404.0268868226; chem.pot.=0.151390; E(RPA)=-404.83147808473; i-freq=None; Gsolv=-5.23935125

C	-3.8941489	1.7860552	-0.4018204
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C	-3.2208889	-0.4074932	0.3138461
C	-4.5547168	-0.8172112	0.2091233
C	-5.5395127	0.0658450	-0.1923805
C	-5.2159256	1.3801879	-0.5050685
H	-3.6263964	2.8103158	-0.6450818
H	-4.8085570	-1.8467336	0.4429149
H	-6.5659702	-0.2763318	-0.2639950
H	-5.9810201	2.0767228	-0.8259267
C	-1.4635977	1.3945905	0.1393078
C	-0.4783687	0.2359114	0.1317194
H	-1.3521050	1.9554277	1.0753542
H	-1.2347202	2.0982234	-0.6659139
C	-0.9465912	-0.8449470	1.0865383
H	-0.4075879	-0.1901976	-0.8737841
H	0.5191836	0.5775959	0.4165576
N	-2.2448320	-1.3200467	0.6667263
H	-0.9695634	-0.4398015	2.1107235
H	-0.2538525	-1.6894710	1.0838797
H	-2.5864993	-2.1337841	1.1511375

1e’
19
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1e’’
19
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oBQ
12
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C	-2.2679466	0.6706163	0.0766474
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oBQH2
14
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H -1.5637896 -2.5794873 -0.1211871

PQ
24
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C -3.8401971 1.5747780 0.1400305
C -2.6576380 0.7126280 -0.0146924
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H -7.5053984 -0.3348184 0.1507629

PQH2
26
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oBQ-dimer
24
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C -2.0450520 0.6398273 1.4884664
C -0.8426027 1.4492814 1.6477370
O -2.9474991 -1.5500990 1.8089525
C -1.9735302 -0.8463833 1.9373297
C 0.2669988 0.9069741 2.1684131
H 1.1638244 1.5073038 2.2738193
C -0.7097585 -1.3175013 2.4978713
C 0.3327467 -0.4819544 2.5996739
H -0.6598789 -2.3536556 2.8105928
H 1.2723184 -0.8351862 3.0100114

PQ-dimer
48
E(PBE0)=-1376.5257085828; chem.pot.=0.313730; E(RPA)=-1378.86179202643; i-freq=None; Gsolv=-18.32624509
C -1.3638760 -2.5371296 -0.4871647
C 0.0276963 -2.9546774 0.0176231
O -2.3101272 -3.2477873 -0.2459117
O 0.1167475 -3.8736195 0.7973285
C -1.4664166 -1.2717386 -1.2279411
C -0.3181567 -0.5562121 -1.6054043
C 1.0261007 -1.0721306 -1.2982070
C 1.1899470 -2.2132676 -0.4949934
C -2.7377395 -0.7830967 -1.5177848
C -2.8962696 0.4242970 -2.1692099
C -1.7689632 1.1463492 -2.5363793

C -0.5007064 0.6607610 -2.2621354
H -3.5925695 -1.3696161 -1.2043581
H -3.8861216 0.8111111 -2.3770934
H -1.8737528 2.1072840 -3.0256938
H 0.3512322 1.2571600 -2.5578679
C 2.4615802 -2.6812908 -0.1716626
C 3.5874726 -2.0399914 -0.6471209
C 3.4363846 -0.9191812 -1.4541852
C 2.1770786 -0.4432930 -1.7723760
H 2.1014852 0.4326957 -2.4013034
H 4.5753173 -2.4096234 -0.4001458
H 4.3097885 -0.4058922 -1.8389895
H 2.5371510 -3.5632012 0.4529668
H 4.5324947 2.4883887 0.4061189
C 3.5508684 2.1015934 0.6515877
H 2.4758210 3.6052267 -0.4516182
C 2.4147076 2.7226114 0.1736064
H 4.2997636 0.4815389 1.8461745
C 3.4181122 0.9789688 1.4593588
O 0.0505763 3.8718569 -0.8011956
C 1.1509625 2.2326147 0.4952535
C 2.1668188 0.4812544 1.7757857
C -0.0233381 2.9532394 -0.0195524
C 1.0058207 1.0894425 1.2991542
H 2.1054542 -0.3952885 2.4054931
C -1.4077884 2.5136536 0.4860683
C -0.3297194 0.5503955 1.6045982
O -2.3654077 3.2091567 0.2455537
C -1.4896179 1.2464993 1.2264445
H 0.3696573 -1.2517732 2.5566917
C -0.4920961 -0.6698292 2.2605907
C -2.7527110 0.7362624 1.5150410
C -1.7521579 -1.1769542 2.5335881
H -3.6171257 1.3083091 1.2011471
C -2.8912494 -0.4739413 2.1658166
H -1.8411072 -2.1397452 3.0223939
H -3.8745588 -0.8776214 2.3726750

1e-oBQ-C
33
E(PBE0)=-785.2136013243; chem.pot.=0.228783;
E(RPA)=-786.63913279907; i-freq=None; Gsolv=-
10.67117876
C -1.6550122 -1.1000811 -1.6028098
C -2.8436228 -1.1094672 -0.7761171
C -0.8313914 -0.0386543 -1.6482450
C -1.1031617 1.1483319 -0.8496211
C -2.3485148 1.1190881 0.0640149
C -3.1863780 -0.0715970 0.0058866
H -4.0748460 -0.0830554 0.6266271
H -3.4684721 -1.9959663 -0.8007001
H -1.4483737 -1.9760571 -2.2064741
H 0.0479839 -0.0172586 -2.2805653
O -0.4144300 2.1498289 -0.8895018
O -2.5921006 2.0710036 0.7764911
C 0.0375753 -2.5769509 0.8114699
C -0.5545900 -1.5719609 1.5604823
C 1.1916459 -2.2901801 0.0854818
C 1.7495935 -1.0273744 0.0624984
C 1.1339776 -0.0013972 0.8151426
C -0.0267171 -0.2953602 1.5547349
H -0.4800318 0.4892659 2.1508580
H 1.6691041 -3.0767383 -0.4915863
C 2.9724337 -0.7158641 -0.7531006
C 3.7011942 0.5069079 -0.2181462
H 2.6773192 -0.5286551 -1.7934644
H 3.6339482 -1.5858176 -0.7736615
C 2.7241945 1.6520908 -0.0428904
H 4.4996377 0.8083938 -0.8991596
H 4.1607026 0.2742268 0.7475170
N 1.6601338 1.2514828 0.8499080
H 2.3179534 1.9519242 -1.0177496
H 3.2210939 2.5231407 0.3892135
H -0.3732782 -3.5792570 0.8099656
H -1.4470234 -1.7751594 2.1401617
H 1.0457016 1.9823780 1.1711061

1e-PQ-C
45
E(PBE0)=-1092.2982014757; chem.pot.=0.320030;
E(RPA)=-1094.27192518431; i-freq=None; Gsolv=-
14.93019684
C 1.5407591 1.8270563 -0.0959262
C 0.3187006 1.9368148 -1.0094603
O 1.9264229 2.8074407 0.5021266
O -0.1809038 3.0245660 -1.1942404
C -0.2023442 0.6998513 -1.6126599
C 0.4465155 -0.5308624 -1.4270437
C 1.7206935 -0.6014059 -0.6959628
C 2.2282249 0.5258296 -0.0308908
C 3.4082832 0.4459337 0.7066104
C 4.1094784 -0.7398889 0.7861154
H 3.7578445 1.3416609 1.2058508
C 3.6312859 -1.8551448 0.1060197
H 5.0270324 -0.7981502 1.3591434
C 2.4591626 -1.7842918 -0.6232294
H 4.1788262 -2.7898564 0.1445262
H 2.1174880 -2.6707445 -1.1396868
C -0.1627029 -1.6730465 -1.9467684
C -1.3544601 -1.5958300 -2.6435300
H 0.2803392 -2.6463324 -1.7890657
C -1.9701998 -0.3681131 -2.8547249
C -1.3900298 0.7718689 -2.3371730
H -1.8083983 -2.5037283 -3.0233364
H -2.8995147 -0.3077964 -3.4082687
H -1.8479009 1.7445259 -2.4711129
C -1.7974365 -2.9471577 1.1568624
C -0.4907199 -2.6965930 1.5521280
C -2.6711530 -1.8809429 0.9983592
C -2.2726358 -0.5684114 1.2054352
C -0.9353362 -0.3219530 1.5509433
C -0.0634976 -1.3968240 1.7477441
H 0.9616430 -1.1980489 2.0422052
H 0.2042957 -3.5151439 1.7015089
H -2.1375269 -3.9620192 0.9884991
H -3.7014165 -2.0686731 0.7111538
C -3.2542631 0.5668717 1.1158363
C -2.5784419 1.9129764 0.9111365
H -3.8404978 0.5918001 2.0427886
H -3.9678037 0.3736433 0.3102460

C -1.3850564 2.0730461 1.8319344
H -3.2835936 2.7262469 1.0952905
H -2.2435255 2.0106988 -0.1214207
N -0.4574653 0.9740716 1.6425695
H -1.7213888 2.1225717 2.8775555
H -0.8532172 3.0008151 1.6084236
H 0.3953284 1.0597012 2.1742537

1e-oBQ-TS1_2C
33
E(PBE0)=-785.1852479188; chem.pot.=0.226322; E(RPA)=-786.59650725375; i-freq=-1255.25; Gsolv=-11.56076436
O 1.5679797 -1.0915102 -1.6871439
H 2.0837658 -0.2407751 -1.0810561
C -0.1845737 -0.5662573 3.1087452
C 0.5968884 -0.2054737 2.0238724
C 0.0650221 0.7020115 1.1011136
C -1.2245607 1.2033001 1.2483675
C -1.9869373 0.8220632 2.3392487
C -1.4678833 -0.0599413 3.2754905
H 0.2202024 -1.2626982 3.8358610
H -1.6211302 1.8877201 0.5070772
H -2.9893211 1.2164347 2.4555440
H -2.0604639 -0.3575499 4.1321837
C 1.9597620 -0.7776909 1.7714452
C 2.8479851 0.2297916 1.0548297
H 1.8625571 -1.6746235 1.1487777
H 2.4164937 -1.0921517 2.7116645
C 2.1542767 0.7936614 -0.1499745
H 3.7923534 -0.2257536 0.7537663
H 3.0932655 1.0564529 1.7362159
N 0.8305983 1.0832429 0.0058284
H 2.6871486 1.5199979 -0.7571485
H 0.4193062 1.7414839 -0.6396742
C -0.6102539 -1.6453859 -0.9709666
C 0.2979258 -0.8421187 -1.7044382
C -0.1816381 0.3231776 -2.4678343
C -1.6102550 0.5491350 -2.4306556
C -2.4370049 -0.2612459 -1.7207583
C -1.9432267 -1.3752378 -0.9817422
O 0.6120955 1.0902890 -3.0320699
H -1.9898360 1.3971536 -2.9900251
H -3.5036610 -0.0616060 -1.7092625
H -2.6364413 -1.9996163 -0.4316212
H -0.2060467 -2.4805680 -0.4095163

1e-oBQ-TS1_4C
33
E(PBE0)=-785.1813032196; chem.pot.=0.226754; E(RPA)=-786.59578010153; i-freq=-1163.12; Gsolv=-10.42677642
O 1.2240022 1.7720833 -0.4307518
H 0.4273451 1.6053486 -1.2466975
C -2.3025970 0.7608480 -0.3550291
C -1.2056040 0.3303094 -1.1368002
C -0.6112226 -0.9433235 -0.8393707
C -1.0987768 -1.6812399 0.2609034
C -2.1428452 -1.2079319 1.0072436
C -2.7735352 0.0113426 0.6832854
H -2.7574778 1.7141970 -0.6013042
H -0.6256365 -2.6249890 0.5072569
H -2.4993866 -1.7877308 1.8502724
H -3.6155712 0.3548871 1.2714541
C -0.6008533 1.1230965 -2.1301017
C 0.1626431 0.4145444 -3.2146104
H -1.1186931 2.0394497 -2.4063637
C 1.0617655 -0.6587938 -2.6360699
H -0.5559235 -0.0291807 -3.9168451
H 0.7742597 1.1136063 -3.7875577
N 0.3658738 -1.4333372 -1.6184549
H 1.9483499 -0.2104609 -2.1815379
H 1.3850792 -1.3461873 -3.4202352
H 0.8938776 -2.2005025 -1.2322273
O 2.4603764 -0.6707945 0.0403143
C 1.6951202 -0.1867344 0.8824099
C 0.9655203 1.0806839 0.6369463
C 0.0557940 1.5545991 1.6102651
C -0.1663008 0.8695553 2.7668400
H -0.4680721 2.4791487 1.3957009
C 0.5591810 -0.3245928 3.0448560
H -0.8699916 1.2480871 3.4984563
C 1.4530178 -0.8251348 2.1591092
H 0.3819230 -0.8375658 3.9843973
H 2.0018757 -1.7392515 2.3559642

1e-PQ-TS1_2C
45
E(PBE0)=-1092.2594830223; chem.pot.=0.316008; E(RPA)=-1094.21824462394; i-freq=-753.53; Gsolv=-15.75379599
O 1.5787013 -1.0709011 -1.7563480
H 2.0854275 -0.3358220 -1.1120734
C -0.4214891 -0.5724914 2.9586325
C 0.4597673 -0.1965718 1.9579297
C 0.0150045 0.7245689 1.0042925
C -1.2707683 1.2540609 1.0574168
C -2.1306988 0.8594263 2.0655650
C -1.7099958 -0.0592053 3.0169204
H -0.0915480 -1.2901818 3.7024275
H -1.5933587 1.9603968 0.3006368
H -3.1343405 1.2656299 2.1012309
H -2.3827926 -0.3746123 3.8052169
C 1.8424774 -0.7679562 1.8370899
C 2.7867398 0.2056008 1.1456116
H 1.7920777 -1.6958982 1.2590923
H 2.2255449 -1.0310094 2.8251025
C 2.1782206 0.7703636 -0.0976043
H 3.7387764 -0.2715947 0.9093868
H 3.0106829 1.0406373 1.8258204
N 0.8635068 1.0835390 -0.0396070
H 2.7668730 1.4297214 -0.7273035
H 0.5082849 1.7332495 -0.7277681
C -0.5768124 -1.6995668 -0.9849723
C 0.2941381 -0.8417924 -1.7398803
C -0.2074542 0.3117637 -2.4515193
C -1.6575720 0.5564346 -2.3645347
C -2.5032181 -0.2656987 -1.5963954
C -1.9567265 -1.4166104 -0.8840385
O 0.5501294 1.1035570 -3.0292836

C -2.1730922 1.6686565 -3.0349112
C -0.0516793 -2.8170568 -0.3196747
C -3.5129806 1.9800901 -2.9624437
H -1.4815849 2.2724787 -3.6101772
C -4.3597073 1.1700887 -2.2066777
H -3.9059986 2.8424162 -3.4881222
C -3.8625011 0.0705794 -1.5389083
H -5.4168723 1.4016667 -2.1416849
H -4.5467781 -0.5358687 -0.9606762
C -0.8538589 -3.6222214 0.4578463
C -2.2103366 -3.3312045 0.5811965
C -2.7471071 -2.2501374 -0.0894405
H -2.8498698 -3.9564123 1.1931542
H 1.0008371 -3.0385918 -0.4426981
H -0.4309891 -4.4801648 0.9679304
H -3.8050997 -2.0505926 0.0175343

1e-PQ-TS1_4C
45
E(PBE0)=-1092.2526675670; chem.pot.=0.316755;
E(RPA)=-1094.21507131013; i-freq=-236.45; Gsolv=-
14.88645257
O 1.2098071 1.7969542 -0.4717308
H 0.4436539 1.6650602 -1.1965268
C -2.2824031 0.6810984 -0.3302201
C -1.1871543 0.2768693 -1.1385311
C -0.5339166 -0.9625706 -0.8220347
C -0.9926218 -1.7182042 0.2841144
C -2.0455581 -1.2809996 1.0326619
C -2.7105450 -0.0723125 0.7173655
H -2.7633453 1.6240906 -0.5646737
H -0.4794325 -2.6395287 0.5351569
H -2.3689931 -1.8631506 1.8871400
H -3.5413522 0.2587333 1.3274871
C -0.6811627 1.0510859 -2.1804860
C 0.1738635 0.3936150 -3.2198917
H -1.2281770 1.9476519 -2.4596211
C 1.1278703 -0.6114945 -2.6040222
H -0.4857080 -0.1057054 -3.9443718
H 0.7520802 1.1290704 -3.7825022
N 0.4561487 -1.4239458 -1.5997996
H 1.9691066 -0.1017101 -2.1282816
H 1.5188481 -1.2810578 -3.3721987
H 1.0199956 -2.1590987 -1.2010441
O 2.4512117 -0.5781596 0.1119939
C 1.6480582 -0.0855231 0.9132267
C 0.9346279 1.1438144 0.6357440
C 0.0456165 1.7205617 1.6026558
C -0.2597763 1.0390299 2.8014116
C -0.5484942 2.9674421 1.3434949
C 0.4235988 -0.2132428 3.1086229
C 1.3673571 -0.7341871 2.2071289
C 2.0395422 -1.9217135 2.5007449
C -1.4565485 3.5132980 2.2180454
H -0.2773108 3.4884185 0.4340477
C -1.7898280 2.8273020 3.3880144
H -1.9077383 4.4754260 2.0038020
C -1.1908806 1.6187480 3.6716897
H -2.5066165 3.2496334 4.0825482
H -1.4524157 1.1162836 4.5937564
C 1.7881177 -2.6080328 3.6689943
H 2.7612361 -2.2827191 1.7780311
C 0.8499593 -2.1023131 4.5674895
H 2.3157201 -3.5287458 3.8894308
C 0.1846702 -0.9259207 4.2911937
H 0.6425233 -2.6300822 5.4915106
H -0.5333499 -0.5569979 5.0117871

1f-oBQ-TS1_2C
37
E(PBE0)=-899.6341303901; chem.pot.=0.256339;
E(RPA)=-901.23474056379; i-freq=-1274.09; Gsolv=-
13.13458693
O 1.6198822 -1.0501115 -1.7594335
H 2.1054876 -0.2138327 -1.0908946
C -0.2793565 -0.6714382 3.0162116
C 0.5203136 -0.2726888 1.9672560
C 0.0102369 0.6568040 1.0498867
C -1.2856308 1.1342818 1.1819968
C -2.0826111 0.7260768 2.2404897
C -1.5783528 -0.1803997 3.1659650
H 0.0908776 -1.3851719 3.7439701
H -1.6762364 1.8341637 0.4522139
H -3.0868434 1.1166913 2.3265664
C 1.8941114 -0.8285509 1.7384223
C 2.7927723 0.2055117 1.0744994
H 1.8181753 -1.7074622 1.0877384
H 2.3266839 -1.1668557 2.6815560
C 2.1324209 0.7887296 -0.1408951
H 3.7512928 -0.2337603 0.7949275
H 3.0056135 1.0179163 1.7833000
N 0.8020050 1.0667218 -0.0150809
H 2.6765575 1.5393294 -0.7072431
H 0.4062197 1.7416458 -0.6527953
C -0.5793519 -1.6267866 -1.1338911
C 0.3507518 -0.8010747 -1.8124858
C -0.1057189 0.3914140 -2.5463498
C -1.5339930 0.6225400 -2.5344803
C -2.3819536 -0.2074961 -1.8730384
C -1.9110228 -1.3497962 -1.1644079
O 0.7025498 1.1764020 -3.0649579
H -1.8963792 1.4921089 -3.0719566
H -3.4476332 -0.0019092 -1.8797507
H -2.6191820 -1.9904903 -0.6532962
H -0.1917810 -2.4829111 -0.5923588
C -3.5862074 -0.1833770 4.4147427
O -2.2657503 -0.6452362 4.2320324
H -3.9571246 -0.6725538 5.3130770
H -4.2229268 -0.4531595 3.5661812
H -3.6121800 0.9018317 4.5560809

1e-oBQ-TS2
47
E(PBE0)=-1167.6412610077; chem.pot.=0.334276;
E(RPA)=-1169.72174899558; i-freq=-153.95; Gsolv=-
17.22488397
C -0.0834985 -0.0677925 0.0062327
N 1.7989821 0.0060925 -0.0018061
C 2.2735614 1.4099714 0.0041033
C 3.3896363 1.6544741 0.9954174

C	3.0125246	1.0704104	2.3474650
C	2.7930454	-0.4027216	2.1897775
C	2.2799163	-0.8897938	0.9869507
C	-0.4454634	0.6510546	1.2531990
C	-1.2223961	1.7356801	1.1856305
C	-1.6257096	2.3000595	-0.0911813
C	-1.1988313	1.8231406	-1.2746964
C	-0.2725873	0.7059488	-1.3120697
C	3.1587633	-1.3210347	3.1642946
C	3.0105866	-2.6846936	2.9589506
C	2.5148135	-3.1514875	1.7507414
C	2.1529370	-2.2554358	0.7591581
O	0.3189643	0.3406443	-2.3098259
O	-0.4022249	-1.2964355	-0.0570820
O	-2.1974169	-1.9583973	1.8030830
C	-3.2800096	-1.1885352	1.5352136
C	-3.6614267	-0.8233340	0.2325245
C	-4.8015432	-0.0503758	0.0521088
C	-5.5781493	0.3503442	1.1282745
C	-5.2086996	-0.0174718	2.4132965
C	-4.0643559	-0.7764055	2.6051808
O	-2.9905282	-1.2159426	-0.8778788
H	2.5740777	1.6612248	-1.0122884
H	1.4216577	2.0435283	0.2672229
H	3.5583432	2.7311950	1.0602478
H	4.3184968	1.1952515	0.6453770
H	3.7939979	1.2498726	3.0881802
H	2.1045270	1.5617253	2.7173280
H	3.5776561	-0.9553968	4.0959352
H	3.2987324	-3.3828497	3.7358230
H	2.4093367	-4.2152211	1.5757205
H	1.7634355	-2.6060350	-0.1878384
H	-0.1958922	0.1704846	2.1926239
H	-1.6055661	2.1952733	2.0890939
H	-2.2957337	3.1527586	-0.0717118
H	-1.4931437	2.2659220	-2.2186735
H	1.8705882	-0.3950041	-0.9348691
H	-1.4800691	-1.8169114	1.1434755
H	-2.0629511	-1.4383496	-0.6726228
H	-3.7521308	-1.0758444	3.5995450
H	-5.8052982	0.2835496	3.2665186
H	-6.4680417	0.9451778	0.9586521
H	-5.0701565	0.2181728	-0.9635041

1e-PQ-TS2
71
E(PBE0)=-1781.7649109540; chem.pot.=0.515443; E(RPA)=-1784.94137515836; i-freq=-75.91; Gsolv=-25.41553888

N	0.0485281	-0.0189595	-0.0322800
C	1.8161696	-0.0046710	-0.0662049
C	2.1330944	1.4723484	-0.0384766
C	2.8980820	2.0399297	0.9873683
C	3.3721134	1.2214257	2.1161826
C	3.0219333	-0.1348153	2.2174567
C	2.2042870	-0.7997026	1.1904005
O	1.8867621	-1.9640296	1.2709601
O	2.1432733	-0.6090931	-1.1558845
C	3.4540385	-0.9083353	3.2948357
C	4.2363848	-0.3573803	4.2870080
C	4.5934922	0.9836412	4.1963473
C	4.1688584	1.7567779	3.1316296
C	3.1887837	3.4057265	0.9136708
C	2.7378674	4.1852027	-0.1334773
C	1.9910951	3.6103666	-1.1516360
C	1.7052198	2.2590860	-1.1018866
C	-0.7437970	0.8323498	0.8368633
C	-2.0842380	0.9391725	0.4679444
C	-2.5161403	0.1416069	-0.7196622
C	-2.0113895	-1.3026047	-0.5908168
C	-0.5780152	-1.3753579	-0.0412322
C	-2.9274622	1.7073960	1.2570702
C	-2.4419690	2.3415329	2.3921859
C	-1.1141827	2.1896268	2.7612940
C	-0.2557825	1.4236214	1.9847602
O	0.6509279	-0.0563102	-3.1742415
C	-0.0697627	-1.1596143	-3.4905935
C	0.3248131	-2.4348289	-3.1886846
C	-0.5058991	-3.5463347	-3.5500268
C	-1.7363296	-3.3421668	-4.2168634
C	-2.1527191	-1.9939091	-4.5243937
C	-1.3116299	-0.9171981	-4.1597701
C	-2.5080245	-4.4697846	-4.5445357
C	-2.0929277	-5.7414535	-4.2282898
C	-0.8781152	-5.9351634	-3.5622763
C	-0.0991704	-4.8545912	-3.2288657
C	-1.7073792	0.4020201	-4.4514154
C	-2.9022495	0.6572613	-5.0786454
C	-3.7411629	-0.4025781	-5.4376903
C	-3.3672197	-1.6973871	-5.1651552
O	1.4812179	-2.7400273	-2.5601590
H	0.0561554	-2.0297814	-0.6314075
H	-0.5574891	-1.7268702	0.9866177
H	-2.6674709	-1.8535822	0.0849551
H	-2.0616463	-1.7901810	-1.5647397
H	-2.1106317	0.5834416	-1.6387293
H	-3.6003236	0.1618675	-0.8311325
H	-3.9734445	1.7976786	0.9850633
H	-3.1076141	2.9420246	3.0009735
H	-0.7387097	2.6640646	3.6597628
H	0.7730813	1.2965102	2.2870474
H	-0.0536786	0.3374668	-0.9872060
H	1.7921325	-2.0192105	-1.9623573
H	1.3740690	-0.2586803	-2.5197169
H	5.2125666	1.4329200	4.9643584
H	4.4735476	2.7933892	3.0983975
H	3.1591078	-1.9500005	3.3227962
H	4.5714642	-0.9604160	5.1220336
H	1.1462468	1.8122173	-1.9157210
H	1.6395466	4.2089194	-1.9833214
H	2.9752811	5.2421199	-0.1575902
H	3.7750184	3.8787805	1.6892849
H	0.8418111	-4.9892502	-2.7126235
H	-0.5509927	-6.9372219	-3.3093543
H	-2.7089801	-6.5922602	-4.4953968
H	-3.4518354	-4.3433566	-5.0588779
H	-1.0469921	1.2139304	-4.1764431
H	-3.1922192	1.6786185	-5.2976409
H	-4.6845713	-0.2063237	-5.9337880
H	-4.0310911	-2.5019304	-5.4536922

1e-oBQ-E
47
E(PBE0)=-1167.6427968339; chem.pot.=0.336157; E(RPA)=-1169.72214395777; i-freq=None; Gsolv=-18.06171629

C	0.3868634	0.7725223	-0.3820680
N	2.0097949	0.9458476	-0.4491729
C	2.4540411	2.0177158	0.5005470
C	3.6739589	1.6423831	1.3061385
C	3.4822999	0.2652193	1.9177300
C	3.3111714	-0.7224740	0.8059678
C	2.6731495	-0.3366688	-0.3689392
C	0.0127202	0.3643948	1.0098153
C	-0.9916831	0.9860553	1.6324225
C	-1.6334537	2.1530994	1.0549125
C	-1.2288781	2.7218811	-0.0963006
C	-0.0821790	2.1843920	-0.7980079
C	3.8541687	-2.0006847	0.8588968
C	3.7596872	-2.8647765	-0.2199551
C	3.1409896	-2.4489959	-1.3898070
C	2.5980876	-1.1779465	-1.4693988
O	0.4859505	2.7381330	-1.7229589
O	0.0074066	-0.0972073	-1.2877767
O	-1.4873298	-2.0262455	-0.2951551
C	-2.6711634	-1.4563771	0.0200852
C	-3.2082512	-0.3631429	-0.6862780
C	-4.4422257	0.1485828	-0.3017565
C	-5.1605468	-0.4075041	0.7460153
C	-4.6371123	-1.4914489	1.4346451
C	-3.3996791	-2.0009034	1.0707932
O	-2.5966075	0.1961228	-1.7539757
H	2.6081066	2.9197018	-0.0882614
H	1.6154862	2.1951171	1.1785715
H	3.8121166	2.4057644	2.0744680
H	4.5679022	1.6443491	0.6762632
H	4.3376564	-0.0185995	2.5329096
H	2.6046809	0.2733838	2.5748143
H	4.3696528	-2.3115558	1.7611935
H	4.1862244	-3.8586940	-0.1540839
H	3.0765503	-3.1132139	-2.2427689
H	2.1007986	-0.8420556	-2.3691657
H	0.4436764	-0.5547845	1.3914095
H	-1.3812852	0.6024291	2.5676559
H	-2.4754049	2.5776543	1.5906385
H	-1.7069334	3.6026771	-0.5072895
H	2.0806496	1.3134134	-1.4020426
H	-0.8707640	-1.3715943	-0.7141293
H	-1.6207781	0.0641186	-1.7142917
H	-2.9676326	-2.8466805	1.5944041
H	-5.1857048	-1.9419564	2.2536751
H	-6.1247297	0.0058728	1.0181487
H	-4.8305023	0.9927603	-0.8608136

1e-PQ-E
71
E(PBE0)=-1781.7805730619; chem.pot.=0.517140; E(RPA)=-1784.95717815259; i-freq=None; Gsolv=-25.12202541

C	1.5337317	2.6568959	-0.5238758
O	2.4839798	3.2321989	-1.0222269
C	0.3169486	3.3328232	-0.0855921
C	-0.6004263	2.6663344	0.7439584
C	-0.3582416	1.2817355	1.1837658
C	0.6862520	0.5254706	0.6332241
C	1.5426832	1.1204833	-0.4523466
N	3.1901731	0.9115025	-0.0333011
C	3.7117145	-0.3961796	-0.3400565
C	3.7555596	-0.7798897	-1.6743782
C	4.1672917	-2.0602420	-2.0039902
C	4.5562049	-2.9406203	-1.0061428
C	4.5584304	-2.5265229	0.3165749
C	4.1379079	-1.2520849	0.6744522
C	4.2010385	-0.7664415	2.0887913
C	4.5247389	0.7166107	2.0823397
C	3.4518183	1.4638229	1.3272568
H	3.7030084	2.5153166	1.1987887
H	2.5130500	1.4036808	1.8817966
H	4.5641889	1.1200735	3.0961360
H	5.5042640	0.8815356	1.6242414
H	4.9541751	-1.3348555	2.6373918
H	3.2426718	-0.9311661	2.5952787
H	4.9030270	-3.1984750	1.0953944
H	4.8810771	-3.9428369	-1.2593858
H	4.1840692	-2.3652267	-3.0430436
H	3.4478316	-0.0827186	-2.4411244
O	1.3476916	0.6454813	-1.6458486
C	0.8198593	-0.8181617	0.9597995
C	0.0975087	4.6455182	-0.5019205
H	3.5430355	1.5866721	-0.7199415
O	0.0893589	-1.6499960	-2.0195636
C	-1.1274854	-1.4818174	-1.4524451
H	0.6363921	-0.8313461	-1.9045575
O	-1.3111532	0.8196880	-2.0766361
H	-0.3300997	0.8004327	-2.0866240
C	-1.7964957	-0.2895247	-1.4719768
C	-1.7054172	-2.6229207	-0.8121840
C	-2.9692283	-2.5331406	-0.1833337
C	-1.0009417	-3.8404402	-0.7846509
C	-3.6627444	-1.2667218	-0.1830006
C	-3.0670662	-0.1578786	-0.8282100
C	-4.8986597	-1.0737817	0.4562852
C	-0.0283871	-1.4154171	1.8737709
H	1.5710214	-1.4155393	0.4617817
C	-1.0394962	-0.6660119	2.4551461
H	0.0786523	-2.4682190	2.1047355
C	-1.2041667	0.6602160	2.1055985
H	-1.7223774	-1.1234089	3.1608272
H	-2.0202152	1.2123625	2.5508971
C	-1.0449652	5.3156061	-0.1197783
H	0.8381184	5.1123818	-1.1397716
C	-1.9692309	4.6629640	0.6898570
H	-1.2260142	6.3300939	-0.4531874
C	-1.7502023	3.3655734	1.1150676
H	-2.8792420	5.1708210	0.9883377
H	-2.5053781	2.8885562	1.7234604
C	-1.5271580	-4.9450989	-0.1608796
H	-0.0315085	-3.8815132	-1.2637857
C	-2.7804069	-4.8665757	0.4565752
H	-0.9729871	-5.8770309	-0.1481899

C -3.4801825 -3.6826673 0.4418492
H -3.2018107 -5.7368459 0.9465989
H -4.4471181 -3.6445394 0.9271971
C -5.5213433 0.1526058 0.4665886
C -4.9248297 1.2445300 -0.1734793
C -3.7189910 1.0887178 -0.8118451
H -5.4137384 2.2124293 -0.1664670
H -3.2413091 1.9248765 -1.3046931
H -5.3773721 -1.9039327 0.9597808
H -6.4743181 0.2698317 0.9698251

1e-oBQ-TS3
47
E(PBE0)=-1167.6283536668; chem.pot.=0.333294; E(RPA)=-1169.71057480045; i-freq=-522.39; Gsolv=-16.79484658
O -0.0890354 0.0066256 -0.0343446
H 1.0584773 0.0093321 -0.0492261
O 2.2642103 0.3957725 -0.0498084
C 2.9810020 0.3891487 -1.1787320
C 2.4531885 -0.0404483 -2.4141775
C 3.2395953 -0.0000937 -3.5563790
C 4.5463206 0.4635867 -3.5134818
C 5.0776550 0.8920421 -2.3066143
C 4.2985941 0.8497448 -1.1602056
O 1.1796918 -0.4970837 -2.5586032
C -0.3993523 1.1001113 0.7230155
C 0.0908099 0.8491920 2.1257465
C -0.7520056 0.5380600 3.1099420
C -2.1847693 0.5815162 2.9071376
C -2.7395309 0.9493418 1.7387786
C -1.9188906 1.3405919 0.6036501
O -2.3851049 1.7872679 -0.4217975
N 0.4188653 2.2854716 0.1644238
C 0.4597371 3.5271474 0.9194987
C -0.4263135 3.8370891 1.9323040
C -0.3216249 5.0743195 2.5528251
C 0.6447659 5.9804228 2.1440461
C 1.5063186 5.6615576 1.1038167
C 1.4247937 4.4279037 0.4749524
C 2.2782052 4.0003009 -0.6743191
C 1.4301373 3.3951119 -1.8049347
C 0.2063431 2.6368216 -1.2865118
H 0.0326665 1.7121706 -1.8283779
H -0.6985597 3.2335931 -1.3269936
H 1.0742022 4.1884822 -2.4637074
H 2.0586463 2.7305690 -2.3993503
H 2.9928431 3.2423874 -0.3311354
H 2.8742476 4.8341291 -1.0448528
H 2.2485280 6.3780440 0.7698040
H 0.7198353 6.9463594 2.6292156
H -1.0064199 5.3278837 3.3526048
H -1.1951618 3.1445312 2.2468946
H 1.1671940 0.7917237 2.2511566
H -0.3744704 0.2416157 4.0809508
H -2.8253486 0.3143891 3.7409446
H -3.8124559 1.0009581 1.5986591
H 1.3735878 1.8199930 0.1767082
H 0.6675812 -0.4123818 -1.7418393
H 2.7968802 -0.3385779 -4.4866713
H 5.1405487 0.4858449 -4.4192451
H 6.0980127 1.2538680 -2.2516647
H 4.6996660 1.1691282 -0.2038518

1e-PQ-TS3
71
E(PBE0)=-1781.7605506862; chem.pot.=0.513083; E(RPA)=-1784.93684436311; i-freq=-339.74; Gsolv=-26.26507992
O -0.1366047 0.2645097 0.2125156
H 0.9904946 0.1735944 0.1503905
O 2.2409328 0.4468732 0.0577183
H 1.4537362 1.9959701 0.3179391
H 0.5395104 -0.3350160 -1.5043080
C 2.8832364 0.3689061 -1.1054525
C 2.2956392 -0.0542943 -2.2719426
C 3.0159258 -0.0784154 -3.5046780
C 4.3641175 0.3510840 -3.5558129
C 4.9998572 0.7998680 -2.3398210
C 4.2599870 0.7887141 -1.1346232
O 0.9959990 -0.4527138 -2.3486320
C -0.3410702 1.4019662 0.9458360
C 0.0794251 1.1824718 2.3937671
C -0.8494862 0.5938229 3.2641061
C -2.2145843 0.2861523 2.8072160
C -2.7060581 0.8729295 1.6340949
C -1.8340319 1.7332630 0.8251864
O -2.2543424 2.5774896 0.0696556
N 0.5299415 2.5053751 0.3167612
C 0.6602244 3.7935340 0.9873343
C -0.1609292 4.2153884 2.0148980
C 0.0377374 5.4789877 2.5505832
C 1.0363751 6.3013095 2.0506439
C 1.8373708 5.8679452 1.0048829
C 1.6597877 4.6049866 0.4575991
C 2.4548391 4.0592132 -0.6832920
C 1.5412228 3.4404621 -1.7522210
C 0.2997529 2.7768601 -1.1551028
H 0.0729578 1.8267901 -1.6295972
H -0.5749956 3.4130592 -1.2085005
H 1.2014776 4.2179186 -2.4380427
H 2.1133809 2.7166222 -2.3331165
H 3.1387432 3.2860918 -0.3122293
H 3.0868864 4.8329785 -1.1188603
H 2.6091387 6.5143258 0.6019928
H 1.1862030 7.2881867 2.4721728
H -0.5962955 5.8178305 3.3605053
H -0.9415986 3.5838530 2.4140863
C 1.3704257 1.4350494 2.8379022
C -3.0725629 -0.5476561 3.5229901
C 2.3842916 -0.5136288 -4.6865013
C 6.3298166 1.2522401 -2.2960571
C 1.7478658 1.1440318 4.1377892
H 2.1146638 1.8556892 2.1758018
C 0.8260803 0.5933570 5.0128270
H 2.7593389 1.3549161 4.4629068
C -0.4570180 0.3219591 4.5747711
H 1.1042016 0.3751843 6.0369918
H -1.1710779 -0.0956687 5.2723781
C -4.3690241 -0.7727656 3.0922059

H -2.7271086 -1.0427319 4.4209242
C -4.8521018 -0.1620368 1.9405972
H -5.0102081 -1.4355154 3.6618113
C -4.0168328 0.6656490 1.2161791
H -5.8672510 -0.3425799 1.6089476
H -4.3541387 1.1509126 0.3082881
C 3.0596904 -0.5294748 -5.8819367
H 1.3535055 -0.8378743 -4.6343063
C 4.3929074 -0.1089171 -5.9384552
H 2.5590384 -0.8696596 -6.7814176
C 5.0242782 0.3211245 -4.7951888
H 4.9293684 -0.1223224 -6.8800900
H 6.0563902 0.6408016 -4.8601098
C 6.9120555 1.6696739 -1.1222639
H 6.9180090 1.2758565 -3.2044402
C 6.1796714 1.6424528 0.0694400
H 7.9403140 2.0126016 -1.1220764
C 4.8770426 1.2072250 0.0589505
H 6.6405137 1.9584135 0.9986004
H 4.2989901 1.1642935 0.9733502

1e-oBQ-F
33
E(PBE0)=-785.2114477867; chem.pot.=0.233351; E(RPA)=-786.64321661634; i-freq=None; Gsolv=-10.82816930
C -2.4866075 -0.0172524 -0.6336773
O -2.7407630 -0.0196902 -1.8242467
C -3.3745200 0.5069180 0.3787902
C -3.1321825 0.2572878 1.6793028
C -1.9996416 -0.5245252 2.1272883
C -1.1121795 -1.0253922 1.2636160
C -1.1572215 -0.6939913 -0.1966182
N -0.0514902 0.2396349 -0.4797136
C 1.2789111 -0.1489561 -0.2066680
C 1.6669998 -1.4973441 -0.2316399
C 2.9716556 -1.8774849 0.0236167
C 3.9463935 -0.9289427 0.2912474
C 3.5791219 0.4040965 0.2891751
C 2.2717538 0.8152260 0.0549669
C 1.9613121 2.2841586 0.0606441
C 0.7115235 2.5575270 -0.7428204
C -0.3879781 1.6412636 -0.2634564
H -1.3039625 1.8600355 -0.8130960
H -0.5903378 1.8394175 0.8006495
H 0.3855281 3.5939890 -0.6325588
H 0.8938956 2.3775867 -1.8065300
H 2.8162455 2.8385774 -0.3343241
H 1.8157532 2.6304331 1.0911720
H 4.3259602 1.1698787 0.4762307
H 4.9723041 -1.2198795 0.4822133
H 3.2239928 -2.9316755 -0.0013375
H 0.9387555 -2.2559987 -0.4686374
O -1.0762894 -1.8631458 -0.9538229
H -1.4015161 -1.6214141 -1.8357639
H -0.2617965 -1.6047961 1.6019106
H -1.8890721 -0.7047652 3.1901419
H -3.8203210 0.6303935 2.4308725
H -4.2511528 1.0484342 0.0443705

1e-PQ-F
45
E(PBE0)=-1092.2942196263; chem.pot.=0.321290; E(RPA)=-1094.27383976543; i-freq=None; Gsolv=-14.52519016
C -0.2133417 -0.5554203 1.5899729
O -0.0427543 -0.7472271 2.7700436
C -0.1739927 -1.5886980 0.5419327
C -1.1264735 -1.5032786 -0.4831361
C -1.0674646 -2.4357796 -1.5120535
C -0.0867341 -3.4183946 -1.5159801
C 0.8384586 -3.5013491 -0.4846813
C 0.7876952 -2.5855413 0.5548050
H 1.5073011 -2.6147609 1.3643035
H 1.6015204 -4.2700650 -0.4957809
H -0.0467422 -4.1275661 -2.3347173
H -1.7830216 -2.3932364 -2.3243107
C -2.1772828 -0.4759825 -0.3711203
C -3.4151576 -0.6165764 -0.9914756
C -4.4059004 0.3390323 -0.8236868
C -4.1778937 1.4406244 -0.0135354
C -2.9503547 1.5903816 0.6175339
C -1.9529298 0.6504427 0.4323475
C -0.5742101 0.8435653 1.0587510
O -0.6192463 1.7481822 2.1265074
H -0.4832035 1.2201152 2.9298057
N 0.3610495 1.2206650 0.0335362
C 1.7182228 0.9293884 0.1638837
C 2.3384956 0.7533171 1.4017499
C 3.6665638 0.3554614 1.4727126
C 4.4113372 0.1734268 0.3199411
C 3.8121426 0.4074196 -0.9122434
C 2.4808343 0.7707557 -1.0065481
C 1.8035948 1.0825450 -2.3003030
C 0.9790696 2.3435126 -2.0790798
C -0.1111362 2.0616181 -1.0639041
H -0.5097060 3.0034574 -0.6686439
H -0.9345008 1.5521741 -1.5716701
H 0.5090448 2.6933355 -3.0009727
H 1.6400338 3.1397742 -1.7249821
H 2.5379423 1.2103282 -3.0979604
H 1.1367389 0.2609746 -2.5929716
H 4.3876411 0.2963295 -1.8261844
H 5.4510633 -0.1262212 0.3757085
H 4.1222254 0.2117922 2.4459750
H 1.7929900 0.9446900 2.3140338
H -2.7537239 2.4414489 1.2570302
H -4.9555105 2.1808272 0.1338395
H -5.3645152 0.2107005 -1.3126329
H -3.6187634 -1.4954661 -1.5914324

1e-oBQ-TS4
33
E(PBE0)=-785.1847943536; chem.pot.=0.231443; E(RPA)=-786.60847662021; i-freq=-129.91; Gsolv=-9.54120888
N 0.2787707 0.5531442 1.1349819
C 1.9781728 -0.6145458 0.3956383
H 1.5239226 2.0138051 0.3125066
O 2.5005889 1.0553099 -1.1254699

C 0.6401419 1.9386066 0.9724655
C 1.8212817 0.0346651 -0.9100685
C 0.8866845 -0.5603299 -1.8176561
C 0.2786883 -1.7276866 -1.4929844
C 0.5830226 -2.4194826 -0.2762313
C 1.4647081 -1.9078906 0.6218260
C -0.9278659 0.1395919 0.6597050
C -1.4568976 -1.0695276 1.1540033
C -2.7057108 -1.5206455 0.7520332
C -3.4435836 -0.7850420 -0.1583405
C -2.9345439 0.4134832 -0.6616438
C -1.6950002 0.8784944 -0.2809607
C -1.1181440 2.1633978 -0.7700064
C -0.4394846 2.8493878 0.4048693
H 0.9793231 2.2986401 1.9496572
H 0.0101001 3.7998226 0.1084886
H -1.1883501 3.0661236 1.1739743
H -1.8949473 2.7877924 -1.2163493
H -0.3732528 1.9624020 -1.5508967
H -3.5235718 0.9955138 -1.3635987
H -4.4224196 -1.1289050 -0.4723140
H -3.1026820 -2.4426119 1.1606715
H -0.8947565 -1.5993156 1.9103913
O 2.9468622 -0.1262851 1.1539555
H 3.2869854 0.6462887 0.6582861
H 1.7250526 -2.4254788 1.5368271
H 0.1301955 -3.3875615 -0.1014047
H -0.4292038 -2.1780815 -2.1790150
H 0.7084557 -0.0651979 -2.7645418

1e-oBQ-G
33
E(PBE0)=-785.1854516041; chem.pot.=0.230483;
E(RPA)=-786.60609849664; i-freq=None; Gsolv=-
9.75497573
H 1.2630368 2.1497175 0.2008493
O 2.4605807 1.2989956 -1.0529638
C 0.3899666 2.0681806 0.8877418
C 1.8963970 0.1910976 -0.8969590
C 0.9595456 -0.4032777 -1.7931315
C 0.3867690 -1.5994939 -1.4880950
C 0.7507781 -2.3105760 -0.3103908
C 1.6975215 -1.8180767 0.5544129
C 2.2073487 -0.5470848 0.3204192
N 0.1642208 0.6840763 1.1581498
C -0.9450969 0.1003303 0.6854896
C -1.2759879 -1.1858595 1.1809412
C -2.4534993 -1.8149069 0.8014752
C -3.2973532 -1.2019171 -0.1051223
C -2.9694365 0.0501012 -0.6402880
C -1.8166390 0.7012158 -0.2762193
C -1.4126788 2.0269857 -0.8221814
C -0.7770846 2.8415370 0.2926541
H 0.7368488 2.5270717 1.8203366
H -0.4266625 3.8086934 -0.0741711
H -1.5249028 3.0366233 1.0691801
H -2.2687737 2.5373406 -1.2684842
H -0.6734668 1.8735070 -1.6203642
H -3.6389945 0.5187259 -1.3546764
H -4.2199965 -1.6865404 -0.4032300
H -2.7083658 -2.7814631 1.2198638
H -0.6361334 -1.6096111 1.9421832
O 3.1210063 0.0037656 1.0988165
H 3.3526623 0.8409134 0.6432859
H 1.9991211 -2.3619416 1.4411988
H 0.3183704 -3.2876853 -0.1351561
H -0.3464196 -2.0378542 -2.1547150
H 0.7141653 0.1316458 -2.7028690

1e-oBQ-TS5
33
E(PBE0)=-785.1831229053; chem.pot.=0.228238;
E(RPA)=-786.59920717251; i-freq=-393.97; Gsolv=-
9.64476448
H 1.4089481 1.8962801 0.1984529
O 2.4363102 1.2192301 -0.6733513
C 0.4562598 2.0275796 0.9085217
C 1.9529235 0.0320545 -0.6416868
C 1.1166669 -0.5220089 -1.6385167
C 0.5405536 -1.7487634 -1.4539345
C 0.8009214 -2.4905985 -0.2829370
C 1.6629486 -2.0203872 0.6832488
C 2.2157431 -0.7555251 0.5275143
N 0.0888635 0.7360800 1.2163995
C -1.0129928 0.1987818 0.6381911
C -1.4464454 -1.0553327 1.1116297
C -2.6084590 -1.6304278 0.6247731
C -3.3345148 -0.9808372 -0.3598717
C -2.8977872 0.2459699 -0.8650063
C -1.7508065 0.8426233 -0.3915192
C -1.2108998 2.1258226 -0.9308736
C -0.5441777 2.9114636 0.1853000
H 0.9219076 2.5023065 1.7791407
H -0.0442424 3.8002332 -0.2046759
H -1.3010810 3.2509553 0.9030120
H -2.0011649 2.7020254 -1.4166464
H -0.4633166 1.8941280 -1.7014590
H -3.4702300 0.7403575 -1.6435322
H -4.2463695 -1.4239457 -0.7435938
H -2.9460206 -2.5836762 1.0138610
H -0.8743524 -1.5197950 1.9035749
O 3.0489311 -0.2450198 1.4280904
H 3.3093336 0.6235170 1.0676451
H 1.8813177 -2.5922440 1.5769393
H 0.3396102 -3.4630966 -0.1588662
H -0.1238345 -2.1587330 -2.2049251
H 0.9272190 0.0655595 -2.5292786

1e-PQ-TS5
45
E(PBE0)=-1092.2506898420; chem.pot.=0.316261;
E(RPA)=-1094.21499568703; i-freq=-892.47; Gsolv=-
13.85614635
H 1.3680811 1.8835993 0.1705029
O 2.2826241 1.2606781 -0.6722074
C 0.4389587 2.0241070 0.9904444
C 1.8550816 0.0446964 -0.6301437
C 1.0334395 -0.5442454 -1.6580379
C 0.4873320 -1.8324199 -1.4756928
C 0.7961941 -2.5799003 -0.2660515

C	1.6307544	-2.0108571	0.7230936
C	2.1283720	-0.6936780	0.5299650
N	0.0729195	0.7372437	1.2524613
C	-1.0354581	0.2293216	0.6266326
C	-1.4826972	-1.0365174	1.0392493
C	-2.5809782	-1.6262826	0.4427070
C	-3.2443348	-0.9659300	-0.5812649
C	-2.8223774	0.2979662	-0.9864456
C	-1.7342026	0.9108544	-0.3988355
C	-1.2484284	2.2638315	-0.8200851
C	-0.5655972	2.9579787	0.3434108
H	0.9934539	2.4597171	1.8277920
H	-0.0710363	3.8759006	0.0194819
H	-1.3110444	3.2388706	1.0982552
H	-2.0795445	2.8580947	-1.2070152
H	-0.5349472	2.1454449	-1.6425025
H	-3.3544991	0.8140017	-1.7793496
H	-4.1011465	-1.4257108	-1.0602996
H	-2.9129726	-2.6050411	0.7683329
H	-0.9465399	-1.5273134	1.8419590
O	2.9445938	-0.1652311	1.4344351
H	3.1954977	0.7054891	1.0766881
C	1.9236553	-2.7160337	1.9017208
C	-0.3540466	-2.3370194	-2.4748345
C	1.4123775	-3.9740994	2.1047341
H	2.5545608	-2.2468052	2.6456125
C	0.6001363	-4.5545817	1.1254064
H	1.6386805	-4.5150442	3.0157999
C	0.3033288	-3.8717737	-0.0318820
H	0.1989950	-5.5500440	1.2770358
H	-0.3317738	-4.3475332	-0.7667372
C	-0.6347394	-1.6087078	-3.6108716
H	-0.8057261	-3.3132131	-2.3606104
C	-0.0699300	-0.3467449	-3.7939645
H	-1.2935708	-2.0236366	-4.3647606
C	0.7569020	0.1755304	-2.8251756
H	-0.2814399	0.2198692	-4.6933277
H	1.2106618	1.1518895	-2.9444879

1f-oBQ-TS5
37
E(PBE0)=-899.6366883351; chem.pot.=0.258116;
E(RPA)=-901.24113335137; i-freq=-479.46; Gsolv=-
11.38681083

H	1.3930842	1.8584732	0.1995767
O	2.4187613	1.2235615	-0.6575945
C	0.4346645	2.0216401	0.9161267
C	1.9550996	0.0194871	-0.6417733
C	1.1206643	-0.5286477	-1.6372480
C	0.5431033	-1.7603003	-1.4591137
C	0.8058367	-2.5061622	-0.2970537
C	1.6761479	-2.0373549	0.6671089
C	2.2313265	-0.7757921	0.5125572
N	0.0427411	0.7434697	1.2350691
C	-1.0461939	0.2115188	0.6494569
C	-1.4911431	-1.0443482	1.1072763
C	-2.6490886	-1.6213995	0.6232058
C	-3.3658665	-0.9629894	-0.3724604
C	-2.9145623	0.2699488	-0.8761580
C	-1.7782082	0.8564262	-0.3913089
C	-1.2243572	2.1337717	-0.9306488
C	-0.5505660	2.9148098	0.1848832
H	0.9159900	2.4959230	1.7778399
H	-0.0383404	3.7942182	-0.2101412
H	-1.3053952	3.2694372	0.8978132
H	-2.0058030	2.7166977	-1.4221520
H	-0.4767700	1.8866140	-1.6960199
H	-3.4922901	0.7431955	-1.6629629
O	-4.4981418	-1.4272350	-0.9203070
H	-2.9795918	-2.5731737	1.0148236
H	-0.9234977	-1.5202317	1.8958363
O	3.0618912	-0.2620256	1.4214679
H	3.3095734	0.6113000	1.0646977
H	1.8975105	-2.6122341	1.5584671
H	0.3431035	-3.4779958	-0.1715668
H	-0.1241257	-2.1629261	-2.2119911
H	0.9227543	0.0656549	-2.5220024
C	-5.0067888	-2.6650135	-0.4620646
H	-5.9159100	-2.8453825	-1.0311931
H	-5.2458230	-2.6216923	0.6042542
H	-4.2951379	-3.4751061	-0.6448633