The role of exchange in systematic DFT errors for some organic reactions: Electronic supplementary information

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Contents

1 Theoretical Procedures

Ab initio and Density Functional Theory calculations were performed with the Gaussian 03 [1], Molpro 2002.6 [2], Gamess-US [3, 4] and Q-Chem 3.1 [5] programs.

For reactions (*i*) and (*ii*) (which involve only radicals and neutral species), the geometries of all species were optimised at the B3LYP/6-31G(d) level. For reactions (*iii*) and (*iv*) (which include anions or cations), all of the geometries were optimised at the B3LYP/6-31+G(d,p) level. Any additional calculations were performed using these optimised geometries. All geometry optimisations were performed with Gaussian 03.

Reference energies for reactions (*i*) and (*ii*) were calculated at the CCSD(T)/cc-pVTZ level. Coupled cluster calculations for Open-shell species were performed using the RHF-UCCSD method [6], with perturbative triples as defined by Bartlett *et al.* [7]. Standard closed-shell CCSD(T) was used for the reference energies of reactions (*iii*) and (*iv*), however the aug-cc-pVTZ basis was used. All coupled cluster reference calculations were performed with Molpro.

In order to assess the accuracy of various methods with respect to the reference energies, single point energies were calculated using HF, MP2, G3(MP2)-RAD [8] and a variety of DFT methods, using the 6-311+G(3df,2p) basis set unless otherwise stated. HF and MP2 calculations used restricted (closed-shell species) or restricted open-shell (radical species) wavefunctions, while DFT calculations used restricted (closed shell species) or unrestricted (radical species) wavefunctions. Gaussian 03 was used for DFT calculations

unless otherwise stated, using the "ultra-fine" pruned (99,590) grid[1, 9]. All DFT calculations that required analysis of components of reaction energies (e.g. the DFT exchange energy) were performed with Q-Chem 3.1, and used an unpruned (99,590) grid for consistency[9]. Gaussian 03 was used for all G3(MP2)-RAD [8] calculations of closed-shell species. For open-shell species, Molpro was used for the coupled-cluster component, while the large-basis second-order Møller-Plesset perturbation theory (MP2) calculations were performed with Gaussian 03.

Most of the DFT methods used have been cited in our previous papers [10, 11, 12], and only the functionals that are new to this paper will be described. SVWN[13, 14] is a pure exchange correlation functional, dependent only on the electron density, with the exchange and correlation components derived from the uniform electron gas. PBE [15, 16] and PW91 [17] are pure generalized-gradient approximation functionals (GGA's) with both exchange and correlation components, and TPSS [18] is a pure meta-GGA, dependent on the kinetic energy density, τ. BR89B94hyb [19, 20], is a hybrid meta-GGA functional which, in addition to being dependent on the kinetic energy density, τ, is dependent on the laplacian of the electron density, $\nabla^2\rho$. It also has a 15.4% admixture of HF exchange. This is a rare example of a functional whose derivation does not involve the uniform electron gas in any way. It has not been used widely due to its troublesome implementation, but analytical representations of the exchange and correlation components of this functional have recently been derived [20], and are implemented in Q-Chem 3.1.

CASSCF/STO-3G calculations for a variety of small molecules were per-

formed with GAMESS-US, for comparison with frozen-core CCSD(T)/STO-3G, CCSD/STO-3G, CCD/STO-3G and MP2/STO-3G correlation energies. Restricted references were used for closed-shell species, and unrestricted references were used for open-shell species. These coupled cluster calculations were performed with Q-CHEM 3.1. The geometries of these species were optimised using the B3LYP/6-31G(d) method, except the anionic species which were optimised at the B3LYP/6-31+G(d,p) level. Geometry optimisations for these species were performed using GAUSSIAN 03.

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2 Tables of Data for Figures 1 and 2

Table S1: Electronic reaction energy errors for reactions (*i*)-(*iv*) at various levels of theory (Figure 1, kJ/mol).[a]

	Neutral			Radicals			Anions			Cations			**MAD**[b]	**MAXD**[c]
	Et	*i*-Pr	*t*-Bu	Et	*i*-Pr	*t*-Bu	Et	*i*-Pr	*t*-Bu	Et	*i*-Pr	*t*-Bu		
G3(MP2)RAD	1.1	2.1	3.2	1.2	2.6	4.8	−2.6	−4.2	−6.3	0.2	−0.3	0.9	2.5	6.3
MP2	2.5	5.3	7.4	2.9	6.5	10.3	0.7	3.9	5.5	−3.2	4.4	6.8	5.0	10.3
HF	−4.2	−9.1	−14.5	−0.1	−3.3	−8.7	−0.3	3.7	10.6	39.1	17.6	8.0	9.9	39.1
SVWN	1.9	2.8	2.2	−11.9	−20.5	−27.4	−1.6	−8.5	−14.5	−57.2	−78.9	−87.3	26.2	87.3
BLYP	−3.5	−8.1	−13.6	−11.4	−22.8	−34.5	−6.3	−16.0	−22.4	−23.0	−56.2	−68.0	23.8	68.0
PBE	−1.9	−4.9	−8.7	−10.5	−20.5	−30.5	−5.8	−15.2	−21.5	−36.6	−63.1	−73.8	24.4	73.8
TPSS	−3.6	−7.7	−11.9	−9.3	−18.8	−28.4	−8.5	−17.3	−21.2	−20.8	−44.8	−54.2	20.5	54.2
MPW1PW91	−2.6	−6.2	−10.6	−10.8	−21.4	−32.1	−6.8	−15.9	−21.2	−33.5	−61.8	−73.2	24.7	73.2
B3LYP	−3.1	−7.1	−11.9	−9.0	−18.2	−27.8	−4.4	−9.8	−13.0	−14.2	−40.7	−51.7	17.6	51.7
B3P86	−2.4	−5.6	−9.3	−8.9	−17.6	−26.1	−4.9	−9.6	−11.4	−22.3	−44.8	−55.5	18.2	55.5
KMLYP	−0.6	−1.9	−4.1	−5.1	−9.8	−14.3	−0.2	0.9	3.5	−8.3	−22.5	−30.9	8.5	30.9
B1B95	−2.5	−5.5	−8.8	−9.2	−17.9	−26.2	−4.8	−9.4	−11.2	−26.1	−43.4	−52.9	18.2	52.9
MPW1B95	−1.9	−4.3	−7.2	−8.4	−16.2	−23.6	−4.0	−8.2	−9.8	−24.7	−40.4	−48.9	16.5	48.9
BB1K	−2.3	−5.0	−8.0	−7.7	−15.0	−21.9	−3.8	−6.3	−5.9	−18.9	−32.8	−41.6	14.1	41.6
MPW1K	−2.4	−5.4	−9.0	−6.3	−13.0	−20.1	−3.8	−5.5	−4.1	−10.8	−27.6	−37.5	12.1	37.5
MPWB1K	−1.8	−4.1	−6.7	−7.1	−13.7	−20.0	−3.3	−5.4	−5.0	−18.0	−30.7	−38.9	12.9	38.9
BR89B94hyb	−2.5	−6.0	−10.5	−5.5	−11.2	−17.3	−3.3	−8.6	−12.8	−18.8	−45.4	−56.4	16.5	56.4
BMK	−1.5	−3.2	−5.3	−5.3	−10.0	−14.1	−2.6	−2.0	0.6	−4.4	−21.1	−27.7	8.1	27.7
M052X	0.4	0.7	0.8	−3.3	−4.6	−4.4	0.4	3.6	8.4	−0.7	−9.4	−11.1	4.0	11.1

[a]DFT calculations were performed self-consistently using the 6-311+G(3df,2p) basis set. The same basis was used for RHF and RMP2 calculations. CCSD(T)/aug-cc-pVTZ reference energies were used for the anionic and cationic reaction series, while CCSD(T)/cc-pVTZ reference energies were used for the neutral and radical reaction series.
[b]Mean Absolute Deviation from CCSD(T).
[c]Maximum Deviation from CCSD(T).

Table S2: Electronic reaction energy errors of various DFT methods for reactions (*i*)-(*iv*), using (RO)HF/6-311+G(3df,2p) densities for the DFT calculations (Figure 2, kJ/mol).[a]

	Neutral			Radicals			Anions			Cations			**MAD**[b]	**MAXD**[c]
	Et	*i*-Pr	*t*-Bu	Et	*i*-Pr	*t*-Bu	Et	*i*-Pr	*t*-Bu	Et	*i*-Pr	*t*-Bu		
SVWN	1.2	1.6	0.8	−6.2	−11.1	−15.4	0.7	−0.8	−3.9	−50.8	−53.1	−60.6	17.2	60.6
BLYP	−3.8	−8.5	−14.0	−7.7	−16.5	−26.0	−3.5	−7.7	−11.7	−17.8	−36.4	−47.5	16.8	47.5
PBE	−2.3	−5.5	−9.4	−6.9	−14.4	−22.3	−3.5	−7.5	−11.4	−30.7	−40.3	−49.6	17.0	49.6
TPSS	−4.0	−8.3	−12.8	−7.0	−14.8	−23.1	−7.0	−12.3	−15.1	−16.3	−25.5	−33.3	15.0	33.3
MPWPW91	−3.0	−6.8	−11.3	−7.4	−15.7	−24.4	−4.6	−8.9	−12.3	−27.5	−39.5	−49.6	17.6	49.6
B3LYP	−3.2	−7.3	−12.2	−6.6	−14.1	−22.2	−2.9	−5.2	−6.7	−10.6	−28.2	−38.7	13.2	38.7
B3P86	−2.6	−5.9	−9.7	−6.6	−13.6	−20.8	−3.8	−5.9	−6.4	−18.3	−30.8	−40.7	13.7	40.7
KMLYP	−0.7	−2.1	−4.3	−3.8	−7.6	−11.5	0.1	2.0	5.1	−6.8	−17.7	−25.8	7.3	25.8
B1B95	−2.7	−5.8	−9.3	−6.6	−13.4	−20.3	−3.9	−6.4	−7.0	−22.5	−30.1	−38.8	13.9	38.8
MPW1B95	−2.1	−4.7	−7.6	−5.9	−12.0	−18.1	−3.1	−5.2	−5.8	−21.4	−28.1	−36.1	12.5	36.1
BB1K	−2.4	−5.2	−8.3	−5.7	−11.7	−17.6	−3.3	−4.5	−3.5	−16.2	−23.6	−31.9	11.2	31.9
MPW1K	−2.5	−5.6	−9.2	−5.1	−11.0	−17.3	−3.2	−3.8	−1.9	−8.4	−20.0	−29.3	9.8	29.3
MPWB1K	−1.9	−4.3	−7.0	−5.2	−10.6	−15.9	−2.7	−3.6	−2.6	−15.6	−22.2	−29.9	10.1	29.9
BR89B94hyb	−2.9	−6.7	−11.2	−5.8	−12.6	−20.0	−1.8	−3.3	−5.3	−15.3	−30.9	−41.3	13.1	41.3
BMK	−1.8	−3.7	−5.7	−3.4	−6.6	−9.5	−2.2	−0.1	4.9	0.1	−12.6	−19.2	5.8	19.2
MO5-2X	0.0	−0.2	−0.5	−2.3	−3.6	−3.6	1.4	5.4	10.6	2.1	−4.7	−6.8	3.4	10.6

[a]DFT calculations were performed on (RO)HF/6-311+G(3df,2p) basis set. The same basis was used for RHF and RMP2 calculations. CCSD(T)/aug-cc-pVTZ reference energies were used for the anionic and cationic reaction series, while CCSD(T)/cc-pVTZ reference energies were used for the neutral and radical reaction series.
[b]Mean Absolute Deviation from CCSD(T).
[c]Maximum Deviation from CCSD(T).

Table S3: CCSD(T) reference energies for the 12 reaction test set (kJ/mol).

	Et	*i*-Pr	*t*-Bu
Neutral	8.5	14.9	18.5
Radicals	−5.2	−9.4	−13.5
Anions	22.7	20.5	−2.0
Cations	−166.7	−232.4	−294.3

[a]No zero-point energy is included. The frozen-core approximation was used. The cc-pVTZ basis was used for the neutral and radical reactions, and the aug-cc-pVTZ basis was used for the anionic and cationic reactions.

3 Optimised geometries

The geometries for 12 reaction test set are included below, together with the geometries of the 17 small molecules in Table 1.

3.1 Geometries Optimised at the B3LYP/6-31G(d) Level for the 12-reaction Test Set

CH_4

C 0.000000 0.000000 0.000000

H 0.631021 0.631021 0.631021

H -0.631021 -0.631021 0.631021

H 0.631021 -0.631021 -0.631021

H -0.631021 0.631021 -0.631021

EtH

C 0.000000 0.000000 0.765382

C 0.000000 0.000000 -0.765382

H 0.000000 1.021073 1.164008

H 0.000000 -1.021073 -1.164008

H 0.884275 0.510537 -1.164008

H -0.884275 -0.510537 1.164008

H 0.884275 -0.510537 1.164008

H -0.884275 0.510537 -1.164008

***i*-PrH**

C 0.000000 0.000000 0.586401

C 0.000000 1.277215 -0.259938

C 0.000000 -1.277215 -0.259938

H -0.884705 1.322339 -0.907284

H 0.884705 -1.322339 -0.907284

H 0.884705 1.322339 -0.907284

H -0.884705 -1.322339 -0.907284

H 0.000000 2.175627 0.368055

H 0.000000 -2.175627 0.368055

H 0.877720 0.000000 1.246941

H -0.877720 0.000000 1.246941

***t*-BuH**

H 0.000000 0.000000 1.473955

C 0.000000 0.000000 0.373379

C 0.000000 1.461749 -0.095985

C -1.265912 -0.730875 -0.095985

C 1.265912 -0.730875 -0.095985

H -0.886306 1.997152 0.265197

H -1.286431 -1.766139 0.265197

H 2.172737 -0.231013 0.265197

H 0.886306 1.997152 0.265197

H -2.172737 -0.231013 0.265197

H 1.286431 -1.766139 0.265197

H 1.316413 -0.760032 -1.192558

H 0.000000 1.520063 -1.192558

H -1.316413 -0.760032 -1.192558

***t*-BuCH$_3$**

C 0.0000000002 -0.0000000001 -1.5403577912

C 0. 0. 0.

C 1.4522632528 0. 0.5134525972

C -0.7261316264 1.25769687 0.5134525969

C -0.7261316265 -1.2576968699 0.5134525971

H -1.0231786387 -0.0000000001 -1.9363621407

H 0.5115893196 0.8860986938 -1.9363621406

H 0.5115893196 -0.886098694 -1.9363621405

H -0.7422800939 1.2856668361 1.6101161186

H -0.2306907743 2.1717655298 0.1631230108

H -1.7654587327 1.285666836 0.1631230107

H -0.742280094 -1.2856668359 1.6101161187

H -1.7654587327 -1.2856668359 0.1631230108

H -0.2306907744 -2.1717655298 0.163123011

H 1.4845601875 0.0000000001 1.6101161189

H 1.9961495071 -0.8860986939 0.1631230111

H 1.9961495071 0.8860986938 0.163123011

Me$^{\bullet}$

C 0.000000 0.000000 0.000000

H 0.000000 1.082752 0.000000

H 0.937691 -0.541376 0.000000

H -0.937691 -0.541376 0.000000

Et$^{\bullet}$

C -0.0014599287 0.7954773663 0.

C 0.0222526364 -0.6939020591 0.

H -0.9948107223 -1.1263631861 0.

H -0.0929966331 1.3519648812 0.9274633127

H -0.0929966331 1.3519648812 -0.9274633127

H 0.5280238711 -1.0935092097 0.8876434386

H 0.5280238711 -1.0935092097 -0.8876434386

***i*-Pr$^\bullet$**

H -1.5741282257 0.3384466025 0.

C -0.4949973207 0.2014373026 0.

C 0.1885698354 -0.059540887 -1.3011394423

C 0.1885698354 -0.059540887 1.3011394423

H -0.3378996345 0.4075090427 -2.1413392395

H -0.3378996345 0.4075090427 2.1413392395

H 1.2217611291 0.3159557584 -1.2963791248

H 1.2217611291 0.3159557584 1.2963791248

H 0.256775568 -1.1397546885 -1.5289592366

H 0.256775568 -1.1397546885 1.5289592366

***t*-Bu$^\bullet$**

H -1.1340543532 1.7616707466 0.

C -1.3291518262 0.6720547343 0.

C -0.0635987604 -0.1288255571 0.

C 0.6742610965 -0.3163631938 1.2896997828

C 0.6742610964 -0.3163631938 -1.2896997829

H -1.9400616179 0.4675010949 0.8885877545

H -1.9400616179 0.4675010949 -0.8885877544

H 1.2835911529 0.5687554926 1.555440113

H -0.0116451147 -0.4829080616 2.1301907067

H 1.3678279377 -1.165692268 1.2415727567

H 1.2835911528 0.5687554926 -1.5554401131

H -0.0116451148 -0.4829080615 -2.1301907067

H 1.3678279377 -1.165692268 -1.2415727567

3.2 Geometries Optimised at the B3LYP/6-31+G(d,p) Level for the 12 Reaction Test Set.

EtH

C 0.000000 0.000000 0.766205

C 0.000000 0.000000 -0.766205

H 0.000000 1.020599 1.164627

H 0.000000 -1.020599 -1.164627

H 0.883864 0.510299 -1.164627

H -0.883864 -0.510299 1.164627

H 0.883864 -0.510299 1.164627

H -0.883864 0.510299 -1.164627

***i*-PrH**

C 0.000000 0.000000 0.586375

C 0.000000 1.278324 -0.259956

C 0.000000 -1.278324 -0.259956

H -0.884438 1.323334 -0.906869

H 0.884438 -1.323334 -0.906869

H 0.884438 1.323334 -0.906869

H -0.884438 -1.323334 -0.906869

H 0.000000 2.176517 0.367466

H 0.000000 -2.176517 0.367466

H 0.877257 0.000000 1.246933

H -0.877257 0.000000 1.246933

***t*-BuH**

C 0.000000 0.000000 0.372111

H 0.000000 0.000000 1.472351

C 0.000000 1.463145 -0.095721

C 1.267121 -0.731572 -0.095721

C -1.267121 -0.731572 -0.095721

H 0.000000 1.522122 -1.191839

H 1.318196 -0.761061 -1.191839

H -1.318196 -0.761061 -1.191839

H -0.885689 1.998404 0.265581

H 0.885689 1.998404 0.265581

H 2.173514 -0.232173 0.265581

H 1.287825 -1.766231 0.265581

H -1.287825 -1.766231 0.265581

H -2.173514 -0.232173 0.265581

***t*-BuCH$_3$**

C 0.889819 0.889819 0.889819

C 0.000000 0.000000 0.000000

C -0.889819 -0.889819 0.889819

C -0.889819 0.889819 -0.889819

C 0.889819 -0.889819 -0.889819

H 1.535685 1.535685 0.283050

H 0.283050 1.535685 1.535685

H 1.535685 0.283050 1.535685

H -1.535685 0.283050 -1.535685

H -1.535685 1.535685 -0.283050

H -0.283050 1.535685 -1.535685

H 0.283050 -1.535685 -1.535685

H 1.535685 -0.283050 -1.535685

H 1.535685 -1.535685 -0.283050

H -1.535685 -1.535685 0.283050

H -0.283050 -1.535685 1.535685

H -1.535685 -0.283050 1.535685

Me$^+$

C 0.000000 0.000000 0.000000

H 0.000000 1.095221 0.000000

H -0.948490 -0.547611 0.000000

H 0.948490 -0.547611 0.000000

Et$^+$

H 0.000000 0.000000 1.062577

C 0.000000 0.691785 -0.063316

C 0.000000 -0.691785 -0.063316

H -0.936530 1.248881 -0.075696

H -0.936530 -1.248881 -0.075696

H 0.936530 1.248881 -0.075696

H 0.936530 -1.248881 -0.075696

***i*-Pr**$^+$

H 0.000000 0.000000 1.549962

C 0.000000 0.000000 0.455381

C 0.000000 1.284450 -0.198020

C 0.000000 -1.284450 -0.198020

H -0.167448 1.261881 -1.275343

H 0.167448 -1.261881 -1.275343

H -0.617104 2.023943 0.330857

H 0.617104 -2.023943 0.330857

H 1.036058 1.658503 -0.008516

H -1.036058 -1.658503 -0.008516

***t*-Bu$^+$**

C -0.945792 -1.118282 0.006674

C 0.001931 0.000000 0.003016

C -0.495793 1.377201 -0.012308

C 1.443922 -0.258253 0.008178

H -0.489792 -2.099000 0.140563

H -1.734398 -0.941057 0.753334

H -1.488493 -1.088477 -0.955631

H 2.062283 0.633465 0.112045

H 1.699431 -1.020035 0.757607

H 1.677951 -0.748890 -0.956071

H 0.107078 2.014826 -0.671437

H -1.562986 1.470020 -0.216521

H -0.296680 1.775002 1.002749

Me$^-$

C 0.000000 0.000000 0.118887

H 0.000000 1.044920 -0.237773

H -0.904927 -0.522460 -0.237773

H 0.904927 -0.522460 -0.237773

Et$^-$

C 0.054657 -0.690190 0.000000

H 0.595266 -1.085517 0.876622

H 0.595266 -1.085517 -0.876622

H -0.931725 -1.236865 0.000000

C 0.054657 0.843041 0.000000

H -0.457348 1.245398 -0.894077

H -0.457348 1.245398 0.894077

***i*-Pr$^-$**

C 0.035300 -0.205840 1.246896

H 0.991101 -0.739542 1.388838

H -0.749560 -1.029931 1.257677

H -0.124094 0.384941 2.162300

C 0.035300 0.657782 0.000000

H -0.870293 1.292456 0.000000

C 0.035300 -0.205840 -1.246896

H -0.124094 0.384941 -2.162300

H 0.991101 -0.739542 -1.388838

H -0.749560 -1.029931 -1.257677

***t*-Bu$^-$**

C 0.000000 1.426758 -0.048202

H -0.884508 1.990467 0.284035

H 0.000000 1.488208 -1.184398

H 0.884508 1.990467 0.284035

C 0.000000 0.000000 0.452770

C 1.235608 -0.713379 -0.048202

C -1.235608 -0.713379 -0.048202

H -1.281541 -1.761240 0.284035

H -2.166049 -0.229227 0.284035

H -1.288826 -0.744104 -1.184398

H 1.281541 -1.761240 0.284035

H 1.288826 -0.744104 -1.184398

H 2.166049 -0.229227 0.284035

3.3 Optimised Geometries of the 17 Small Molecules of Table 1.

These molecules were optimised at the B3LYP/6-31G(d) level, except for the anions, which were optimised at the B3LYP/6-31+g(d,p) level.

H_2

H 0. 0. -0.021397166

H 0. 0. 0.721397166

LiH

Li 0. 0. -0.3107366373

H 0. 0. 1.3107366373

BeH_2

H -0.4576949156 0. -0.3078130541

Be 0.315662844 0. 0.7748398815

H 1.0875506471 0. 1.858541327

BH_3

B 0.1199673281 -0.2077895075 0.0848297112

H -0.0795233707 0.1377385185 1.2100814384

H 1.1143679309 0.1377385185 -0.4783358324

H -0.6764690215 -0.8962016781 -0.4783358324

CH_4

C 0.000000 0.000000 0.000000

H 0.631021 0.631021 0.631021

H -0.631021 -0.631021 0.631021

H 0.631021 -0.631021 -0.631021

H -0.631021 0.631021 -0.631021

NH_3

N -0.0222262971 0.0384970758 -0.0157163654

H 0.0089690319 -0.0155348189 1.0020199445

H 0.9477031408 -0.0155348189 -0.3255505638

H -0.4603980226 -0.8285024046 -0.3255505638

H_2O

H 0.0612705972 0. 0.0580162272

O -0.034584112 0. 1.0220325092

H 0.8796213018 0. 1.3425695253

HF

H 0. 0. -0.1167753102

F 0. 0. 0.8167753102

CH_3^+

C 0.000000 0.000000 0.000000

H 0.000000 1.095221 0.000000

H -0.948490 -0.547611 0.000000

H 0.948490 -0.547611 0.000000

NH_4^+

N 0. 0. 0.

H 0. 0. 1.0292180113

H 0.9703560468 0. -0.3430726704

H -0.4851780234 -0.8403529873 -0.3430726704

H -0.4851780234 0.8403529873 -0.3430726704

H_3O^+

O 0. 0. -0.0007330616

H 0. 0. 0.9811021343

H 0.8503168989 0. -0.4916845364

H -0.850316899 0. -0.4916845363

CH_3^-

C 0.000000 0.000000 0.118887

H 0.000000 1.044920 -0.237773

H -0.904927 -0.522460 -0.237773

H 0.904927 -0.522460 -0.237773

OH^-

O 0. 0. 0.0150510299

H 0. 0. 0.9849489701

NH_2^-

N -0.0336531079 0. -0.0237963408

H 0.0258730266 0. 1.0071045261

H 0.9581315952 0. -0.3113081853

$CH_3^{\bullet}$

C 0.000000 0.000000 0.000000

H 0.000000 1.082752 0.000000

H 0.937691 -0.541376 0.000000

H -0.937691 -0.541376 0.000000

$NH_2^{\bullet}$

N -0.0183123493 0. -0.0138628398

H 0.0141372141 0. 1.0199986328

H 0.9855542201 0. -0.2632108489

$OH^{\bullet}$

O 0. 0. 0.0085425324

H 0. 0. 0.9914574676