Long Distance Structural Consequences of H–Bonding. How H–Bonding Affects Aromaticity of the Ring in Variously Substituted Aniline/Anilinium/Anilide Complexes with Bases and Acids.

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Supporting Information

General Information	S2
Tables S1. Geometrical parameters of 4–X–aniline derivatives and their H-bonded complexes (results B3LYP/6-311+G**).	S4
Tables S2. Geometrical parameters of 4–X–aniline derivatives and their H-bonded complexes (results MP2/aug-cc-pVDZ)	S6
Figure S1. Interrelations between α angle, C–N and a bond lengths for MP2 optimized geometry of p-substituted aniline derivatives and their H-bonded complexes.....	S8
Figure S2. Scatter plot of HOMA vs. C–N bond length for MP2 optimized geometry of 4-substituted aniline, anilide anion and anilinium cation, and their H-bonded complexes.....	S9
Table S3. The values of the H-bond interaction energy, BSSE correction, d_{CN} and $d_{\text{N...F}}$ for B3LYP modeling interaction of aniline as $\text{NH}^- \dots \text{HF}$, $\text{NH}_2 \dots \text{F}^-$ and $\text{NH}_2 \dots \text{HF}$ systems	S10
Table S4. Regression equations, correlation coefficients and statistical detail of CSD data	S11
XYZ coordinates of 4–X–aniline, 4–X–anilinium cation and 4–X–anilide anion and their H-bonded complexes	S12
Supplementary References	S20

General Information

B3LYP/6-311+G** and MP2/aug-ccpVDZ levels of theory were employed to optimize the molecules geometries of aniline, anilide and anilinium derivatives substituted in para position (X=NO, NO₂, CN, CHO, H, CH₃, OCH₃, OH) and their H-bonded complexes (only for X=NO, NO₂, CHO, H, OH) with B (B=F⁻, CN⁻) or HB (HB=HF, HCN). In H-bonded complexes the linearity of N...H...B was assumed. All ab initio calculations were performed using the *Gaussian03* series of programs¹. The optimized molecules correspond to minima (no imaginary frequencies). Geometrical parameters of the ring, the C–N bond lengths, d_{CN} , the interatomic distance $d_{\text{N...B}}$ for systems under discussion from B3LYP are presented in Table S1, whereas some MP2 results are shown in Table S2, Figures S1 and S2. The B3LYP optimized geometries are reported on pages S11–S18.

The values of the BSSE correction (B3LYP) for H-bonded complexes, which H-bond interaction energy (eq. 2) is presented in Figure 2, and same geometrical parameters are collected in Table S3.

In this case of the hydrogen bond energy, E , for $\text{PhNH}_2 \cdots \text{F}^- \rightarrow \text{PhNH}_2 + \text{F}^-$ calculated at both computational levels, for their optimal geometry, at 298 K:

$$\text{BSSE}_{\text{B3LYP}} = 1.56 \text{ kcal/mol}, \quad \text{BSSE}_{\text{MP2}} = 2.26 \text{ kcal/mol}$$

$$\text{ZPE}_{\text{B3LYP}} = 1.71 \text{ kcal/mol}, \quad \text{ZPE}_{\text{MP2}} = 1.69 \text{ kcal/mol}$$

No scaling was applied to obtained frequencies for the calculation of thermodynamic parameters.

(1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R.L.; Fox, D.J.; Keith, T.; Al-Laham, M.A.; Peng, C.Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian 03, Revision C.02*, Gaussian, Inc., Wallingford CT, 2004.

Geometries of 332 H-bonded complexes of variously substituted aniline and anilinium cation derivatives with various oxygen and nitrogen acids/bases were retrieved from CSD.² The data were retrieved for mono- and polysubstituted aniline/anilinium cation (substituents: halogen, -Me, -CN, -COOH, -COO⁻, -COOMe, -COOEt, -CONH₂, -CF₃, -NH₂, -NH₃⁺, -NO₂, -OH, -OMe, -SO₃⁻, -H) interacting with N or O atom in acid/base partner. Sometimes solvent molecules were present in the crystal lattice. REFCODE, chemical name, chemical formula moiety and references of retrieved hits are presented in Supplementary References.

In the case of the crystallographic data three kinds of H-bonded interaction were found:

- (i) NH₃⁺...B interactions for anilinium derivatives (Chart 1(i)).
- (ii) NH₂...HB interactions for aniline derivatives (HB is a Broensted acid, Chart 1(ii)).
- (iii) NH₂...B interactions for aniline derivatives (B is a Broensted base, Chart 1(iii)).

Interrelations between α angle, C-N and a bond lengths (for labeling see Chart 3) for retrieved variously substituted aniline/anilinium cation derivatives in their H-bonded complexes are presented in Figure 7, whereas Table S4 gives statistical parameters for them. Student's t -distribution was used to check a significance of the slope of the regression line. There was no data selection except restrictions specified in the Methodology.

The distributions of a and C-N bond lengths as well as α angle values do not form distribution with any features of the normal one. However, the deviations from the regression lines, due to the least square procedure of their estimation, are very close to the normal distribution. Thus, when we test the null hypothesis that correlation coefficient is zeroth and can accept the alternative hypothesis at a given level of significance, we may state, that the lines describing the data is not by chance, and can assume the physically sound interpretation, i.e. the above mentioned data follow the Bent – Walsh rule.

(2) Allen, F. H. The Cambridge Structural Database: a Quarter of a Million Crystal Structures and Rising. *Acta Crystallogr., Sec. B: Struct. Sci.* **2002**, 58 (3 PART 1), 380–388.

Table S1. Geometrical parameters (B3LYP results) of the ring and C–N bond lengths, d_{CN} , for (a) 4–X–aniline, 4–X–anilide anion and 4–X–anilinium cation (X=NO, NO₂, CN, CHO, H, CH₃, OCH₃, OH), and (b) their H-bonded complexes (only for X=NO, NO₂, CHO, H, OH).

(a)	X		$a/\text{\AA}$	$b/\text{\AA}$	$c/\text{\AA}$	α/deg	β/deg	γ/deg	δ/deg	$d_{\text{CN}}/\text{\AA}$
	NO	NH ₂	1.412	1.380	1.403	119.09	120.30	120.28	119.74	1.374
	NO ₂	NH ₂	1.409	1.383	1.395	118.75	120.67	119.51	120.89	1.378
	CN	NH ₂	1.407	1.384	1.404	118.56	120.70	120.61	118.82	1.383
	CHO	NH ₂	1.409	1.383	1.403	118.82	120.33	120.95	118.61	1.382
	H	NH ₂	1.403	1.391	1.395	118.59	120.48	120.78	118.88	1.398
	CH ₃	NH ₂	1.401	1.391	1.398	118.10	120.62	121.74	117.19	1.401
	OCH ₃	NH ₂	1.400	1.392	1.397	117.96	121.16	120.36	118.98	1.407
	OH	NH ₂	1.400	1.392	1.394	118.04	121.04	120.31	119.25	1.406
	NO	NH [–]	1.457	1.364	1.428	114.94	122.21	121.56	117.54	1.314
	NO ₂	NH [–]	1.455	1.367	1.419	114.54	122.59	120.81	118.66	1.315
	CN	NH [–]	1.452	1.372	1.422	114.05	122.72	121.77	116.97	1.320
	CHO	NH [–]	1.455	1.368	1.424	114.36	122.36	122.18	116.57	1.318
	H	NH [–]	1.447	1.385	1.406	113.59	122.71	121.98	117.04	1.332
	CH ₃	NH [–]	1.445	1.386	1.407	113.23	122.76	122.73	115.80	1.334
	OCH ₃	NH [–]	1.447	1.387	1.399	113.52	122.89	121.15	118.39	1.334
	OH	NH [–]	1.446	1.388	1.397	113.45	122.90	121.20	118.33	1.335
	NO	NH ₃ ⁺	1.390	1.391	1.394	123.72	117.85	119.33	121.92	1.497
	NO ₂	NH ₃ ⁺	1.388	1.392	1.389	123.46	118.16	118.70	122.84	1.496
	CN	NH ₃ ⁺	1.388	1.390	1.402	123.16	118.26	119.60	120.32	1.496
	CHO	NH ₃ ⁺	1.388	1.391	1.398	123.43	117.87	120.25	120.32	1.497
	H	NH ₃ ⁺	1.387	1.394	1.394	123.34	117.90	120.17	120.52	1.498
	CH ₃	NH ₃ ⁺	1.387	1.392	1.401	122.69	118.11	121.37	118.35	1.497
	OCH ₃	NH ₃ ⁺	1.389	1.387	1.406	122.23	118.87	120.19	119.66	1.494

	OH	NH ₃ ⁺	1.389	1.388	1.402	122.35	118.73	120.06	120.06	1.494
(b)	X	$d_{N...B}/\text{\AA}$	$a/\text{\AA}$	$b/\text{\AA}$	$c/\text{\AA}$	α/deg	β/deg	γ/deg	δ/deg	$d_{CN}/\text{\AA}$
NH ⁻ ...HF ^a	NO	2.471	1.446	1.367	1.422	116.11	121.61	121.35	117.98	1.323
NH ₂ ...CN ⁻	NO	2.890	1.429	1.372	1.414	118.00	120.66	120.96	118.75	1.339
NH ⁻ ...HF ^a	NO ₂	2.468	1.443	1.370	1.413	115.74	121.98	120.58	119.14	1.324
NH ₂ ...CN ⁻	NO ₂	2.895	1.426	1.376	1.405	117.65	121.02	120.18	119.94	1.341
NH ⁻ ...HF ^a	CHO	2.449	1.441	1.372	1.418	115.79	121.64	121.93	117.08	1.328
NH ₂ ...CN ⁻	CHO	2.929	1.424	1.377	1.411	117.72	120.69	121.55	117.80	1.345
NH ₂ ...F ⁻	H	2.450	1.425	1.388	1.401	116.27	121.41	121.54	117.83	1.349
NH ₂ ...CN ⁻	H	3.030	1.414	1.390	1.398	117.49	120.90	121.20	118.32	1.370
NH ₂ ...F ⁻	OH	2.476	1.419	1.392	1.393	116.11	121.75	120.73	118.93	1.360
NH ₂ ...CN ⁻	OH	3.052	1.410	1.392	1.392	117.40	121.35	120.51	119.15	1.381
NH ₂ ...HF	NO	2.713	1.403	1.384	1.400	119.98	119.96	119.89	120.33	1.412
NH ₂ ...HCN	NO	3.330	1.407	1.383	1.401	119.57	120.13	120.01	120.14	1.398
NH ₂ ...HF	NO ₂	2.710	1.401	1.387	1.392	119.66	120.30	119.15	121.44	1.414
NH ₂ ...HCN	NO ₂	3.317	1.404	1.385	1.393	119.23	120.49	119.28	121.23	1.400
NH ₂ ...HF	CHO	2.700	1.401	1.386	1.401	119.76	119.94	120.63	119.09	1.417
NH ₂ ...HCN	CHO	3.297	1.404	1.385	1.401	119.32	120.14	120.74	118.92	1.404
NH ₂ ...HF	H	2.671	1.397	1.392	1.394	119.59	120.03	120.52	119.32	1.428
NH ₂ ...HCN	H	3.223	1.399	1.392	1.394	119.16	120.23	120.61	119.17	1.417
NH ₂ ...HF	OH	2.657	1.395	1.391	1.394	118.97	120.62	120.13	119.52	1.433
NH ₂ ...HCN	OH	3.204	1.398	1.392	1.394	118.57	120.81	120.21	119.41	1.423

^a In this case the quinoid canonical structure (Chart 2) is dominant.

Table S2. Geometrical parameters (MP2 results) of the ring and C–N bond lengths, d_{CN} , for (a) 4–X–aniline, 4–X–anilide anion and 4–X–anilinium cation (X=NO, NO₂, CN, CHO, H, CH₃, OCH₃, OH), and (b) their H-bonded complexes (only for X=NO, NO₂, CHO, H, OH).

(a)	X		$a/\text{\AA}$	$b/\text{\AA}$	$c/\text{\AA}$	α/deg	β/deg	γ/deg	δ/deg	$d_{\text{CN}}/\text{\AA}$
	NO	NH ₂	1.417	1.398	1.410	119.20	120.50	119.62	120.56	1.397
	NO ₂	NH ₂	1.414	1.401	1.403	118.77	120.95	118.83	121.67	1.400
	CN	NH ₂	1.413	1.401	1.412	118.71	120.85	119.98	119.64	1.402
	CHO	NH ₂	1.415	1.400	1.411	119.01	120.45	120.35	119.39	1.401
	H	NH ₂	1.412	1.405	1.407	118.85	120.48	120.55	119.11	1.412
	CH ₃	NH ₂	1.411	1.406	1.410	118.40	120.61	121.45	117.59	1.413
	OCH ₃	NH ₂	1.410	1.406	1.409	118.26	121.12	120.06	119.40	1.417
	OH	NH ₂	1.411	1.406	1.405	118.34	120.97	120.03	119.66	1.417
	NO	NH [–]	1.460	1.383	1.432	115.10	122.69	120.66	118.16	1.332
	NO ₂	NH [–]	1.456	1.388	1.422	114.56	122.78	120.30	119.37	1.335
	CN	NH [–]	1.454	1.393	1.424	113.95	123.01	121.22	117.70	1.341
	CHO	NH [–]	1.457	1.388	1.428	114.48	122.15	122.05	117.25	1.336
	H	NH [–]	1.451	1.403	1.416	113.55	122.99	121.71	117.21	1.350
	CH ₃	NH [–]	1.450	1.404	1.416	113.18	123.13	122.25	116.20	1.352
	OCH ₃	NH [–]	1.451	1.405	1.409	113.50	123.25	120.65	118.88	1.352
	OH	NH [–]	1.450	1.406	1.408	113.34	123.28	120.76	118.72	1.353
	NO	NH ₃ ⁺	1.403	1.404	1.406	124.00	117.62	119.18	122.21	1.492
	NO ₂	NH ₃ ⁺	1.401	1.405	1.403	123.56	118.16	118.58	123.07	1.492
	CN	NH ₃ ⁺	1.401	1.404	1.414	123.45	118.09	119.80	120.77	1.491
	CHO	NH ₃ ⁺	1.402	1.405	1.410	123.77	117.67	120.09	120.71	1.492
	H	NH ₃ ⁺	1.400	1.407	1.408	123.74	117.63	120.24	120.53	1.492
	CH ₃	NH ₃ ⁺	1.399	1.406	1.413	123.21	117.74	121.38	118.55	1.491
	OCH ₃	NH ₃ ⁺	1.400	1.403	1.416	122.83	118.45	120.15	119.97	1.489

	OH	NH ₃ ⁺	1.400	1.403	1.412	122.91	118.33	120.06	120.32	1.489
(b)	X	$d_{N...B}/\text{\AA}$	$a/\text{\AA}$	$b/\text{\AA}$	$c/\text{\AA}$	α/deg	β/deg	γ/deg	δ/deg	$d_{CN}/\text{\AA}$
NH ⁻ ...HF ^a	NO	2.486	1.450	1.386	1.428	116.16	121.78	120.84	118.60	1.337
NH ₂ ...CN ⁻	NO	2.872	1.433	1.391	1.420	118.15	120.80	120.36	119.52	1.351
NH ⁻ ...HF ^a	NO ₂	2.478	1.446	1.391	1.417	115.68	122.26	119.96	119.88	1.340
NH ₂ ...CN ⁻	NO ₂	2.880	1.429	1.396	1.409	117.69	121.27	119.50	120.78	1.355
NH ⁻ ...HF ^a	CHO	2.463	1.446	1.391	1.423	115.85	121.83	121.35	117.81	1.343
NH ₂ ...CN ⁻	CHO	2.903	1.430	1.395	1.417	117.91	120.80	120.95	118.61	1.357
NH ₂ ...F ⁻	H	2.454	1.432	1.404	1.412	116.47	121.50	121.24	118.06	1.359
NH ₂ ...CN ⁻	H	3.001	1.421	1.405	1.410	117.87	120.87	120.88	118.63	1.385
NH ₂ ...F ⁻	OH	2.485	1.427	1.407	1.405	116.43	121.78	120.32	119.38	1.372
NH ₂ ...CN ⁻	OH	3.022	1.418	1.407	1.405	117.58	121.25	120.15	119.62	1.395
NH ₂ ...HF	NO	2.696	1.412	1.400	1.409	120.11	120.06	119.38	121.01	1.424
NH ₂ ...HCN	NO	3.253	1.415	1.399	1.409	119.69	120.24	119.48	120.86	1.412
NH ₂ ...HF	NO ₂	2.696	1.409	1.402	1.402	119.68	120.50	118.62	122.08	1.426
NH ₂ ...HCN	NO ₂	3.244	1.412	1.402	1.402	119.27	120.68	118.71	121.93	1.414
NH ₂ ...HF	CHO	2.689	1.411	1.401	1.410	119.92	119.99	120.17	119.76	1.427
NH ₂ ...HCN	CHO	3.244	1.413	1.401	1.410	119.50	120.19	120.24	119.65	1.415
NH ₂ ...HF	H	2.674	1.408	1.406	1.407	119.82	119.96	120.40	119.46	1.433
NH ₂ ...HCN	H	3.212	1.411	1.406	1.407	119.40	120.17	120.45	119.36	1.423
NH ₂ ...HF	OH	2.663	1.407	1.405	1.406	119.32	120.45	119.95	119.88	1.437
NH ₂ ...HCN	OH	3.197	1.409	1.406	1.406	118.91	120.65	120.00	119.78	1.427

^a In this case the quinoid canonical structure (Chart 2) is dominant.

Figure S1. Interrelations between (a) α and C–N bond length, d_{CN} , (b) a and C–N bond length, (c) a bond length and α for MP2 optimized geometry of 4-substituted aniline, anilide anion and anilinium cation, and their H-bonded complexes. Ph means C₆H₄

Figure S2. Scatter plot of HOMA vs. C–N bond length, d_{CN} , for MP2 optimized geometry of 4-substituted aniline, anilide anion and anilinium cation, and their H-bonded complexes. Ph means C₆H₄.

Table S3. The values of H-bond interaction energy, E_{int} , BSSE correction, C–N bond length, d_{CN} , and interatomic distance between the nitrogen and fluorine, $d_{\text{N...F}}$, for B3LYP modeling interaction ($d_{\text{N...F}}$ constrained) of aniline as $\text{NH}^- \dots \text{HF}$, $\text{NH}_2 \dots \text{F}^-$ and $\text{NH}_2 \dots \text{HF}$ systems.

Complex	$d_{\text{N...F}} / \text{\AA}$	$d_{\text{CN}} / \text{\AA}$	BSSE /kcal	$E_{\text{int}} / \text{kcal/mol}$
PhNH ⁻ ...HF	4.0	1.335	0.18	-11.42
	3.8	1.336	0.21	-13.24
	3.6	1.336	0.23	-15.50
	3.4	1.337	0.28	-18.28
	3.2	1.337	0.33	-21.70
	3.0	1.338	0.43	-25.90
	2.8	1.340	0.54	-31.15
	2.6	1.341	0.71	-39.00
PhNH ₂ ...F ⁻	4.0	1.384	0.81	-11.99
	3.8	1.383	0.88	-13.82
	3.6	1.381	0.96	-16.03
	3.4	1.379	1.04	-18.69
	3.2	1.376	1.12	-21.86
	3.0	1.371	1.24	-25.58
	2.8	1.365	1.36	-29.94
	2.6	1.356	1.44	-35.50
	2.5	1.352	1.51	-39.59
	2.450 ^a	1.349	1.56	-42.49
PhNH ₂ ...HF	4.0	1.409	0.23	-2.91
	3.8	1.410	0.29	-3.65
	3.6	1.412	0.35	-4.64
	3.4	1.415	0.42	-5.89

3.2	1.417	0.53	-7.37
3.0	1.421	0.69	-9.00
2.8	1.425	0.87	-10.47
2.671 ^a	1.428	0.99	-11.00

^a Fully optimized complex, i.e. without the $d_{N...F}$ interatomic distance constrained.

Table S4. Regression equations, correlation coefficients (cc) and statistical coefficients for significance of the slope of the regression line (Student's t -distribution, t_{calc}) for dependences of (a) α on C–N bond length, d_{CN} , (b) a on C–N bond length, d_{CN} , and (c) a bond length on α angle (n = number of observations, CSD data).

						t_{calc}	$t_{n-2,0.01}$
(a)	$n=332$	$\alpha =$	62.61	$+ d_{\text{CN}} \cdot 40.3 (\pm 3.7)$	$cc =$	0.91	2.338
(i) $\text{NH}_3^+ \dots \text{B}$	$n=220$	$\alpha =$	44.72	$+ d_{\text{CN}} \cdot 52.5 (\pm 18.4)$	$cc =$	0.36	2.344
(ii) $\text{NH}_2 \dots \text{HB}^*$	$n=34$	$\alpha =$	96.30	$+ d_{\text{CN}} \cdot 16.2$	$cc =$	0.27	2.449
(iii) $\text{NH}_2 \dots \text{B}$	$n=78$	$\alpha =$	59.81	$+ d_{\text{CN}} \cdot 42.4 (\pm 7.3)$	$cc =$	0.80	2.376
(b)	$n=332$	$a =$	1.784	$+ d_{\text{CN}} \cdot -0.28 (\pm 0.05)$	$cc =$	-0.86	2.338
(i) $\text{NH}_3^+ \dots \text{B}^*$	$n=220$	$a =$	1.241	$+ d_{\text{CN}} \cdot 0.094$	$cc =$	0.08	2.344
(ii) $\text{NH}_2 \dots \text{HB}$	$n=34$	$a =$	2.084	$+ d_{\text{CN}} \cdot -0.49 (\pm 0.24)$	$cc =$	-0.59	2.449
(iii) $\text{NH}_2 \dots \text{B}$	$n=78$	$a =$	1.809	$+ d_{\text{CN}} \cdot -0.29 (\pm 0.05)$	$cc =$	-0.79	2.376
(c)	$n=332$	$a =$	2.036	$+ \alpha \cdot -0.0054 (\pm 0.0008)$	$cc =$	-0.75	2.338
(i) $\text{NH}_3^+ \dots \text{B}$	$n=220$	$a =$	1.092	$+ \alpha \cdot 0.0024 (\pm 0.0011)$	$cc =$	0.28	2.344
(ii) $\text{NH}_2 \dots \text{HB}^*$	$n=34$	$a =$	1.033	$+ \alpha \cdot 0.0030$	$cc =$	0.22	2.449
(iii) $\text{NH}_2 \dots \text{B}$	$n=78$	$a =$	1.991	$+ \alpha \cdot -0.0050 (\pm 0.0011)$	$cc =$	-0.71	2.376

*Regression line is statistically insignificant, by use Student test at significance level 0.01.

XYZ coordinates of 4-X-aniline, 4-X-anilinium cation, 4-X-anilide anion and their H-bonded complexes; B3LYP/6-311+G** results

aniline $E=-287.687628$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.402970
C	1.198895	0.000000	2.108725
C	2.421734	-0.001451	1.438191
C	2.425291	-0.003072	0.043659
C	1.231807	-0.003163	-0.671360
N	-1.201182	-0.057197	-0.713193
H	-0.944839	-0.004339	1.937629
H	1.175059	0.001516	3.193107
H	3.353165	-0.000829	1.991395
H	3.365978	-0.003956	-0.496306
H	1.249239	-0.009958	-1.756828
H	-2.016545	0.280925	-0.223635
H	-1.161277	0.279148	-1.664068

anilineH+ $E=-288.034437$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.387082
C	1.232094	0.000000	2.038739
C	2.415402	0.001056	1.301309
C	2.380968	0.000496	-0.092216
C	1.158709	0.000959	-0.762379
N	-1.318409	0.028394	-0.710583
H	-0.922981	-0.000529	1.957454
H	1.261830	-0.004064	3.121084
H	3.368808	-0.001330	1.815128
H	3.301399	-0.003202	-0.662447
H	1.127464	0.001064	-1.846994
H	-1.679014	0.984166	-0.813235
H	-1.238963	-0.374062	-1.649843
H	-2.024778	-0.516411	-0.205327

4-NO-aniline $E=-417.022243$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.415617
C	1.185875	0.000000	2.116098
C	2.410244	-0.000625	1.425109
C	2.417695	-0.001845	0.024510
C	1.231048	-0.002098	-0.684993
N	-1.187183	-0.037727	-0.690429
H	-0.947753	-0.002920	1.944577
H	1.199364	0.001573	3.199373
N	3.682605	0.001551	2.052333
H	3.374668	-0.001698	-0.485123
H	1.240160	-0.006087	-1.769702
H	-2.042048	0.175674	-0.202903
H	-1.185824	0.172576	-1.675220
O	3.678410	0.002379	3.275157

4-NO-anilineH+ $E=-417.347120$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.392971
C	1.225396	0.000000	2.044107
C	2.399258	-0.000408	1.287319
C	2.377686	-0.000828	-0.102817
C	1.152837	-0.000703	-0.769420
N	-1.322397	0.001123	-0.700861
H	-0.925194	0.000176	1.960318
H	1.290143	-0.000022	3.125940
N	3.742452	-0.000716	1.891000
H	3.314594	-0.001500	-0.647685
H	1.117406	-0.001061	-1.853857
H	-1.869836	0.840528	-0.477472
H	-1.198016	-0.020460	-1.718150
H	-1.888101	-0.816382	-0.444659
O	3.743855	-0.000523	3.091444

4-NO2-aniline $E=-492.256060$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.408912
C	1.189704	0.000000	2.114372
C	2.399949	-0.001806	1.420737
C	2.425971	-0.003238	0.026018
C	1.235245	-0.003322	-0.677689
N	-1.184955	-0.042294	-0.701348
H	-0.943041	-0.002210	1.944588
H	1.198147	0.002010	3.195735
N	3.657429	0.001196	2.165164
H	3.378103	-0.003742	-0.486680
H	1.251251	-0.008080	-1.762130
H	-2.035625	0.199622	-0.219070
H	-1.170901	0.196769	-1.679818
O	4.705956	0.002477	1.524204
O	3.599720	0.002366	3.392724

4-NO2-anilineH+ $E=-492.578530$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.386943
C	1.227694	0.000000	2.045528
C	2.389598	0.000046	1.286794
C	2.382124	0.000079	-0.103001
C	1.158718	0.000052	-0.765636
N	-1.317112	-0.000079	-0.710098
H	-0.921186	-0.000032	1.959876
H	1.289176	-0.000024	3.125631
N	3.707038	0.000066	1.995323
H	3.317926	0.000126	-0.645861
H	1.128364	0.000067	-1.849814
H	-2.093731	0.000160	-0.040910
H	-1.427588	0.828604	-1.306259
H	-1.427701	-0.829050	-1.305832
O	4.704382	0.000067	1.296385
O	3.674069	0.000063	3.212655

4-CN-aniline $E=-379.957725$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.406508
C	1.190270	0.000000	2.113209
C	2.421983	-0.000996	1.439159
C	2.425093	-0.002720	0.035091
C	1.235322	-0.002863	-0.672453
N	-1.188515	-0.048162	-0.706143
H	-0.943280	-0.003507	1.942261
H	1.174655	0.001687	3.196314
C	3.648577	0.001151	2.168015
H	3.368912	-0.003145	-0.496484
H	1.254890	-0.008574	-1.757075
H	-2.029353	0.226125	-0.222733
H	-1.165681	0.224326	-1.676275
N	4.642803	0.002351	2.759587

4-CN-anilineH+ $E=-380.284478$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.387556
C	1.224656	0.000000	2.045821
C	2.417421	0.001386	1.308033
C	2.382576	0.001140	-0.093811
C	1.161441	0.001590	-0.758914
N	-1.315581	0.028863	-0.711677
H	-0.921725	-0.001036	1.959490
H	1.258348	-0.003768	3.127609
C	3.675757	-0.000948	1.989575
H	3.306517	-0.001729	-0.657502
H	1.136112	0.001738	-1.843378
H	-1.647474	0.988975	-0.865099
H	-1.251909	-0.425572	-1.628822
H	-2.038436	-0.465929	-0.178224
N	4.689186	-0.002832	2.541324

4-CHO-aniline $E=-401.049937$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.406500
C	1.198060	0.000000	2.102110
C	2.426803	-0.000465	1.428737
C	2.424009	-0.001566	0.024036
C	1.235969	-0.002455	-0.680168
N	-1.186933	-0.046345	-0.705623
H	-0.943664	-0.003570	1.942005
H	1.185679	0.001358	3.187951
C	3.683753	0.002344	2.188125
H	3.374981	-0.001178	-0.496079
H	1.245431	-0.007605	-1.765416
H	-2.031922	0.215836	-0.223144
H	-1.165768	0.215696	-1.678487
O	4.798743	0.004774	1.705499
H	3.552436	0.002413	3.292136

4-CHO-anilineH+ $E=-401.381700$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.385377
C	1.233595	0.000000	2.036307
C	2.417717	0.000261	1.299244
C	2.379178	0.000291	-0.100904
C	1.161074	0.000102	-0.766408
N	-1.315526	0.002946	-0.713901
H	-0.922260	-0.000001	1.957133
H	1.266216	-0.000475	3.120254
C	3.744118	-0.000146	2.000898
H	3.313268	0.000074	-0.650191
H	1.127019	0.000061	-1.851000
H	-1.432523	0.844179	-1.290553
H	-1.414304	-0.812283	-1.329759
H	-2.093778	-0.021660	-0.047466
O	4.792309	-0.000142	1.410186
H	3.696781	0.000342	3.106755

4-CH3-aniline $E=-327.014168$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.400817
C	1.197642	0.000000	2.109791
C	2.436129	-0.004041	1.461265
C	2.425080	-0.001300	0.062430
C	1.236286	-0.000865	-0.659972
N	-1.199980	-0.056975	-0.720877
H	-0.943829	0.000677	1.937505
H	1.163452	0.005778	3.195071
C	3.731553	-0.039591	2.237160
H	3.366724	0.002809	-0.478200
H	1.264327	-0.002429	-1.745402
H	-2.011964	0.294332	-0.234402
H	-1.151320	0.292304	-1.666972
H	4.532857	0.473912	1.699532
H	3.624458	0.438869	3.214019
H	4.064752	-1.068828	2.413104

4-CH3-anilineH+ $E=-327.365639$ hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.386572
C	1.227654	0.000000	2.042417
C	2.434933	-0.001349	1.330741
C	2.381954	0.001906	-0.069722
C	1.166985	0.002703	-0.748793
N	-1.313099	0.034820	-0.717658
H	-0.923280	0.002851	1.956903
H	1.243203	-0.000925	3.125973
C	3.755898	-0.033638	2.052555
H	3.302366	0.002691	-0.641694
H	1.148360	0.007619	-1.833860
H	-1.635339	0.994525	-0.888155
H	-1.249785	-0.435694	-1.625952
H	-2.041233	-0.444002	-0.178215
H	4.539724	0.455497	1.472331
H	3.690611	0.454438	3.026146
H	4.069167	-1.068843	2.223228

4-OCH3-aniline E=-402.240663 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.395877
C	1.193895	0.000000	2.121820
C	2.418484	-0.000857	1.454636
C	2.428288	-0.002018	0.056067
C	1.240026	-0.003597	-0.658275
N	-1.200718	-0.063616	-0.729754
H	-0.943102	-0.004858	1.933322
H	1.145774	0.001289	3.202632
O	3.647330	0.000908	2.066037
H	3.382626	-0.002493	-0.457095
H	1.270862	-0.012464	-1.743347
H	-2.010031	0.293022	-0.241619
H	-1.145700	0.315526	-1.664503
C	3.690533	-0.005960	3.482908
H	4.746213	-0.007958	3.750909
H	3.213176	0.886306	3.904957
H	3.211772	-0.901553	3.896052

4-OCH3-anilineH+ E=-402.595684 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.384019
C	1.216708	0.000000	2.062336
C	2.418934	-0.000111	1.339259
C	2.385472	-0.000111	-0.069750
C	1.179166	0.000001	-0.743285
N	-1.305412	0.000080	-0.725558
H	-0.924924	-0.000074	1.952184
H	1.214270	0.000122	3.142858
O	3.640324	-0.000265	1.885727
H	3.323699	-0.000095	-0.609483
H	1.167438	-0.000077	-1.828354
H	-1.414436	0.827921	-1.322205
H	-1.414877	-0.828093	-1.321670
H	-2.086302	0.000507	-0.062569
C	3.785762	-0.000156	3.313683
H	4.857524	-0.000065	3.493581
H	3.340302	0.898118	3.749148
H	3.340393	-0.898413	3.749269

4-OH-aniline E=-362.931602 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.398681
C	1.195892	0.000000	2.114976
C	2.417798	-0.001996	1.446189
C	2.431371	-0.003678	0.052295
C	1.237569	-0.004160	-0.659166
N	-1.203186	-0.063494	-0.725010
H	-0.942128	-0.005086	1.937458
H	1.168357	0.001983	3.200981
O	3.630729	-0.000563	2.097353
H	3.383383	-0.004988	-0.464951
H	1.265875	-0.012544	-1.744209
H	-2.009295	0.302911	-0.238957
H	-1.148953	0.302902	-1.664777
H	3.485335	-0.007032	3.048510

4-OH-anilineH+ E=-363.283343 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.386171
C	1.218998	0.000000	2.055718
C	2.416138	0.000004	1.329450
C	2.386996	0.000038	-0.074436
C	1.175731	0.000011	-0.744748
N	-1.308188	-0.000079	-0.721560
H	-0.923508	0.000030	1.956243
H	1.234060	-0.000067	3.139693
O	3.632212	-0.000007	1.904016
H	3.323208	0.000031	-0.617613
H	1.161237	0.000069	-1.829671
H	-1.419062	0.827459	-1.318384
H	-1.420117	-0.828900	-1.316417
H	-2.086642	0.001211	-0.055666
H	3.577812	0.000132	2.867387

4-NO-anilide HF E=-516.993678 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.442315
C	1.171414	0.000000	2.149084
C	2.437806	-0.000031	1.504010
C	2.462308	-0.000033	0.081487
C	1.301210	-0.000007	-0.637800
N	-1.140110	-0.000085	-0.670707
H	-0.961369	0.000038	1.943256
H	1.165781	0.000017	3.235013
N	3.552049	-0.000054	2.310667
H	3.430191	-0.000046	-0.407374
H	1.330129	-0.000001	-1.725372
H	-2.474790	0.001713	-0.144907
H	-0.996123	0.000128	-1.676688
O	4.672608	-0.000104	1.748292
F	-3.439312	0.003013	0.235068

4-NO-aniline HF E=-517.516581 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.406736
C	1.193499	0.000000	2.101958
C	2.405744	-0.002929	1.397427
C	2.409671	-0.010990	0.000328
C	1.212630	-0.010643	-0.699633
N	-1.224754	-0.054186	-0.700966
H	-0.944178	-0.006244	1.941586
H	1.215428	0.002749	3.184906
N	3.694237	0.002962	2.020437
H	3.362640	-0.016637	-0.516098
H	1.211575	-0.024928	-1.784092
H	-2.001197	0.353478	-0.191757
H	-1.176523	0.343619	-1.632479
O	3.691569	0.015975	3.237242
H	-1.735390	-1.719584	-0.980433
F	-2.009876	-2.614800	-1.130657

4-NO-aniline CN- E=-509.953760 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.425874
C	1.188443	0.000000	2.115133
C	2.432140	-0.000623	1.443890
C	2.441923	-0.001751	0.029355
C	1.264342	-0.001549	-0.672218
N	-1.153197	0.000089	-0.680986
H	-0.954149	0.000294	1.938734
H	1.200207	0.000279	3.200060
N	3.572399	-0.000962	2.241370
H	3.400136	-0.002999	-0.477000
H	1.272263	-0.002789	-1.758772
H	-2.112691	0.004024	-0.214137
H	-1.121443	0.000723	-1.688671
O	4.667453	-0.001482	1.657407
C	-3.751924	0.010746	0.583445
N	-4.803642	0.015059	1.095166

4-NO-aniline HCN E=-510.480317 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.403532
C	1.201448	0.000000	2.093487
C	2.414175	-0.002244	1.397831
C	2.421506	-0.006891	-0.005194
C	1.226595	-0.007142	-0.695970
N	-1.204139	-0.059697	-0.707776
H	-0.941308	-0.001102	1.942698
H	1.226581	0.003151	3.177223
N	3.591868	0.002772	2.204907
H	3.372327	-0.008814	-0.524286
H	1.223406	-0.013564	-1.781364
H	-2.009664	0.301486	-0.213297
H	-1.162215	0.297482	-1.653563
O	4.649080	0.002793	1.599370
H	-1.652054	-2.250248	-0.987096
C	-1.866039	-3.296754	-1.120537
N	-2.094629	-4.414688	-1.263087

4-NO2-anilide HF E=-592.227114 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.442337
C	1.163269	0.000000	2.164588
C	2.418831	-0.003186	1.512836
C	2.460851	-0.007599	0.102795
C	1.299817	-0.006580	-0.626736
N	-1.144384	0.008207	-0.666554
H	-0.961570	0.002748	1.942663
H	1.144725	0.001982	3.246658
N	3.619261	-0.004717	2.262598
H	3.426965	-0.012182	-0.385143
H	1.345641	-0.010328	-1.712486
H	-2.466921	-0.026416	-0.128219
H	-1.006228	0.002135	-1.673043
O	4.713631	-0.003835	1.659123
O	3.556350	-0.005876	3.509457
F	-3.429995	-0.051628	0.263798

4-NO2-aniline HF E=-592.750755 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.400737
C	1.197126	0.000000	2.100351
C	2.395939	-0.000745	1.392735
C	2.417551	-0.007328	0.000827
C	1.217190	-0.008559	-0.693177
N	-1.221357	-0.058788	-0.709873
H	-0.939488	-0.008058	1.942197
H	1.215222	0.001631	3.181412
N	3.668189	0.007868	2.132270
H	3.365900	-0.011501	-0.518450
H	1.222713	-0.022927	-1.777450
H	-2.001040	0.348685	-0.205444
H	-1.167394	0.344754	-1.638666
O	4.706228	0.006737	1.480249
O	3.615275	0.017330	3.356926
H	-1.718252	-1.724016	-0.996455
F	-1.985885	-2.620927	-1.150812

4-NO2-aniline CN- E=-585.187712

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.426345
C	1.181323	0.000000	2.129999
C	2.413773	0.000932	1.451820
C	2.441124	0.000343	0.049527
C	1.262080	-0.000048	-0.661198
N	-1.157836	-0.000123	-0.677135
H	-0.954040	-0.000071	1.939361
H	1.180016	-0.000394	3.211694
N	3.644447	-0.000195	2.189748
H	3.397394	0.000102	-0.456141
H	1.286214	-0.000739	-1.746409
H	-2.111360	0.000135	-0.202509
H	-1.133448	0.000705	-1.684632
O	4.715071	0.004789	1.562501
O	3.596211	-0.005198	3.427669
C	-3.749710	0.000578	0.612994
N	-4.796816	0.000862	1.134201

4-NO2-aniline HCN E=-585.714283

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.404132
C	1.193956	0.000000	2.107127
C	2.397405	0.000561	1.405858
C	2.421804	0.005092	0.012980
C	1.225611	0.006126	-0.685731
N	-1.206474	0.060783	-0.707263
H	-0.940813	0.001826	1.943766
H	1.207246	-0.002093	3.188348
N	3.664031	-0.004910	2.148364
H	3.372138	0.005665	-0.502901
H	1.236569	0.012345	-1.770249
H	-1.694980	2.229575	-0.986456
H	-1.165506	-0.301604	-1.651097
H	-2.010067	-0.302183	-0.210959
O	4.705822	-0.011079	1.500793
O	3.608039	-0.005193	3.373721
C	-1.929752	3.271874	-1.120633
N	-2.180475	4.384996	-1.263928

aniline F- E=-387.627941

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.426025
C	1.184848	0.000000	2.143721
C	2.434900	0.000847	1.506073
C	2.454517	0.003822	0.108521
C	1.277104	0.004563	-0.630479
N	-1.166238	-0.021695	-0.677751
H	-0.961815	0.005157	1.927158
H	1.138483	0.001513	3.230264
H	3.356122	0.000954	2.078724
H	3.406599	0.006590	-0.417621
H	1.321825	0.006354	-1.717296
H	-2.196803	0.125905	-0.178468
H	-1.089597	0.061461	-1.681212
F	-3.353409	0.291556	0.381879

aniline HF E=-388.187161

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.396773
C	1.205350	0.000000	2.093530
C	2.419021	-0.003850	1.408181
C	2.415677	-0.009603	0.014410
C	1.214563	-0.008298	-0.689681
N	-1.233000	-0.056820	-0.717196
H	-0.941330	-0.007568	1.936801
H	1.192874	0.001020	3.177546
H	3.355312	-0.004358	1.953218
H	3.352136	-0.015949	-0.531711
H	1.219354	-0.022130	-1.774853
H	-1.993893	0.383849	-0.210703
H	-1.164951	0.370998	-1.634851
H	-1.757909	-1.661091	-1.018444
F	-2.050532	-2.555430	-1.186382

aniline CN- E=-380.601068

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.414590
C	1.193635	0.000000	2.122631
C	2.430578	-0.002414	1.467975
C	2.441054	0.001297	0.072312
C	1.253430	0.003773	-0.652234
N	-1.179565	-0.046797	-0.694938
H	-0.953953	0.012290	1.929225
H	1.158981	0.005832	3.208248
H	3.357637	-0.002452	2.030593
H	3.386822	0.004182	-0.462545
H	1.281938	0.005321	-1.738695
H	-2.068439	0.226693	-0.222155
H	-1.135067	0.196925	-1.672524
C	-3.760805	0.747401	0.677999
N	-4.758993	1.054524	1.208926

aniline HCN E=-381.149709

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.399436
C	1.202682	0.000000	2.100342
C	2.419902	-0.005377	1.421049
C	2.420100	-0.010489	0.027170
C	1.222027	-0.008857	-0.681830
N	-1.221050	-0.065009	-0.716026
H	-0.942487	-0.001371	1.937998
H	1.185470	0.003369	3.184433
H	3.354105	-0.006295	1.969511
H	3.358421	-0.015571	-0.516037
H	1.233237	-0.017252	-1.767284
H	-1.998921	0.347939	-0.215263
H	-1.162431	0.341326	-1.642295
H	-1.645143	-2.145620	-0.993989
C	-1.859385	-3.196694	-1.134410
N	-2.087200	-4.314366	-1.283727

4-CHO-anilide HF E=-501.012266

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.439132
C	1.173520	0.000000	2.150160
C	2.444160	-0.000089	1.519223
C	2.460850	-0.000816	0.101521
C	1.299671	-0.000636	-0.628079
N	-1.144812	0.001018	-0.672437
H	-0.961077	-0.000322	1.940983
H	1.136617	0.000097	3.237982
C	3.649241	-0.000739	2.302749
H	3.425500	-0.001351	-0.396467
H	1.338845	-0.001529	-1.715182
H	-2.429065	-0.001149	-0.148332
H	-1.008741	-0.000188	-1.678480
O	4.813351	-0.001326	1.894881
H	3.464782	-0.000758	3.403461
F	-3.411945	-0.002808	0.252784

4-CHO-aniline HF E=-501.545925

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.398573
C	1.205271	0.000000	2.087803
C	2.423576	-0.000194	1.400285
C	2.415075	-0.005412	-0.001906
C	1.217816	-0.007686	-0.696347
N	-1.223714	-0.058748	-0.711894
H	-0.940158	-0.009059	1.939643
H	1.202614	0.000533	3.173292
C	3.694184	0.007491	2.151135
H	3.362027	-0.008059	-0.528693
H	1.216265	-0.021118	-1.781358
H	-1.996847	0.367732	-0.212748
H	-1.162597	0.338632	-1.643037
O	4.797693	0.020160	1.650046
H	3.577047	0.001526	3.255791
H	-1.742119	-1.710098	-0.966954
F	-2.023760	-2.607250	-1.105523

4-CHO-aniline CN- E=-493.976520

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.422873
C	1.190212	0.000000	2.116087
C	2.439341	-0.000002	1.458505
C	2.440296	-0.000012	0.047989
C	1.262252	-0.000021	-0.663296
N	-1.159507	0.000047	-0.681648
H	-0.953943	-0.000005	1.936568
H	1.170538	-0.000005	3.203100
C	3.669699	0.000007	2.225115
H	3.395482	-0.000024	-0.466160
H	1.279835	-0.000017	-1.749589
H	-2.106477	-0.000156	-0.210585
H	-1.133559	-0.000137	-1.688561
O	4.812685	0.000012	1.782221
H	3.512194	0.000010	3.328046
C	-3.781559	-0.000514	0.622672
N	-4.829282	-0.000738	1.143854

4-CHO-aniline HCN E=-494.509242

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.401784
C	1.202275	0.000000	2.094587
C	2.424704	0.000722	1.413420
C	2.419633	-0.001527	0.010497
C	1.226098	-0.004331	-0.688571
N	-1.208650	-0.065790	-0.711171
H	-0.941501	-0.003202	1.941109
H	1.195291	0.000935	3.180202
C	3.690399	0.006285	2.168713
H	3.368388	-0.000776	-0.513293
H	1.230471	-0.010340	-1.773889
H	-2.007012	0.310699	-0.215650
H	-1.161379	0.308732	-1.650447
O	4.797591	0.016827	1.674092
H	3.567725	0.000703	3.272968
H	-1.637594	-2.227772	-0.970427
C	-1.845951	-3.277943	-1.096359
N	-2.068225	-4.398259	-1.230702

4-OH-aniline F- E=-462.870576

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.419895
C	1.186679	0.000000	2.143413
C	2.424756	0.006090	1.498690
C	2.459267	0.015096	0.109549
C	1.273768	0.012280	-0.624228
N	-1.177097	-0.041280	-0.679745
H	-0.959824	0.011152	1.924314
H	1.145885	0.001283	3.232206
O	3.637242	0.004460	2.199823
H	3.419802	0.024713	-0.396231
H	1.325151	0.016499	-1.710096
H	-2.149657	0.202005	-0.160379
H	-1.112613	0.148226	-1.669202
H	3.431101	0.039178	3.138154
F	-3.309714	0.492192	0.459115

4-OH-aniline HF E=-463.432293

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.393557
C	1.200360	0.000000	2.101218
C	2.416185	-0.005535	1.419307
C	2.421771	-0.011456	0.024527
C	1.222092	-0.010157	-0.676612
N	-1.233821	-0.061942	-0.725880
H	-0.939188	-0.009047	1.936795
H	1.182412	0.001679	3.186825
O	3.630176	-0.004512	2.056302
H	3.370247	-0.019049	-0.498309
H	1.239308	-0.024834	-1.761540
H	-1.984617	0.416575	-0.238297
H	-1.149428	0.347648	-1.650751
H	3.499917	-0.021711	3.009888
H	-1.782793	-1.650857	-0.972721
F	-2.092355	-2.546837	-1.111914

4-OH-aniline CN- E=-455.844917

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.409759
C	1.192673	0.000000	2.126118
C	2.422185	0.001135	1.468522
C	2.446705	0.006700	0.078427
C	1.254269	0.005993	-0.642550
N	-1.188939	-0.056651	-0.699424
H	-0.951701	0.015199	1.928112
H	1.159354	0.005869	3.213801
O	3.636448	-0.000668	2.150363
H	3.402435	0.012803	-0.434549
H	1.291933	0.006971	-1.728304
H	-2.050303	0.258692	-0.206503
H	-1.143748	0.259777	-1.656846
H	3.450152	0.025409	3.093437
C	-3.713387	0.867543	0.745207
N	-4.682558	1.222354	1.299822

4-OH-aniline HCN E=-456.394385

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.396013
C	1.198288	0.000000	2.107596
C	2.416968	-0.005194	1.431301
C	2.426156	-0.009351	0.036832
C	1.228874	-0.008194	-0.668971
N	-1.222400	-0.072445	-0.725827
H	-0.940166	-0.003855	1.938121
H	1.176202	0.003028	3.193281
O	3.629660	-0.003535	2.073299
H	3.376091	-0.013971	-0.483599
H	1.252017	-0.016617	-1.754117
H	-1.990065	0.380571	-0.243089
H	-1.146025	0.322656	-1.656171
H	3.495209	-0.021458	3.026215
H	-1.693750	-2.129966	-0.915426
C	-1.934660	-3.181578	-1.012331
N	-2.190528	-4.298485	-1.115253

4-NO-PhNH(-) E=-416.468792 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.458380
C	1.148344	0.000000	2.189861
C	2.432567	-0.000223	1.556404
C	2.464401	-0.002015	0.133087
C	1.320437	-0.002346	-0.613954
N	-1.144604	0.001669	-0.644337
H	-0.973376	0.000737	1.939712
H	1.127347	0.000094	3.274148
N	3.634286	0.000412	2.205230
H	3.443073	-0.003330	-0.339682
H	1.372192	-0.003898	-1.700719
H	-0.961468	0.000772	-1.650641
O	3.619336	0.001144	3.467805

4-NO2-PhNH(-) E=-491.701968 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.453523
C	1.151043	0.000000	2.188373
C	2.421733	-0.002609	1.553119
C	2.473680	-0.004855	0.137162
C	1.324554	-0.003949	-0.604640
N	-1.140153	0.003309	-0.654866
H	-0.968469	0.001844	1.942453
H	1.121993	0.001481	3.270594
N	3.602567	-0.003011	2.310128
H	3.446392	-0.007254	-0.338539
H	1.384335	-0.005481	-1.690661
H	-0.949386	0.002403	-1.659518
O	4.712563	-0.005522	1.722101
O	3.530148	-0.000721	3.563520

4-CN-PhNH(-) E=-379.391430 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.451000
C	1.153252	0.000000	2.191115
C	2.438920	0.001656	1.578788
C	2.476053	0.000209	0.159933
C	1.326975	-0.001650	-0.592173
N	-1.142442	0.004121	-0.660767
H	-0.968129	0.000331	1.941562
H	1.094947	-0.001085	3.276082
C	3.622589	0.011058	2.343859
H	3.442962	0.000117	-0.336172
H	1.397769	-0.003896	-1.677914
H	-0.946252	0.008510	-1.664167
N	4.602094	0.018840	2.977695

4-CHO-PhNH(-) E=-400.484108 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.451745
C	1.159885	0.000000	2.177680
C	2.446595	-0.000828	1.566636
C	2.475679	-0.001231	0.143220
C	1.327882	-0.000830	-0.601209
N	-1.138900	0.000723	-0.662762
H	-0.968338	0.000570	1.942437
H	1.108647	0.000520	3.265857
C	3.634459	-0.001001	2.361395
H	3.447700	-0.001679	-0.341808
H	1.385101	-0.000883	-1.688497
H	-0.939681	-0.000234	-1.665828
O	4.813040	-0.001835	1.978320
H	3.430911	-0.000379	3.460552

PhNH(-) E=-287.090175 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.446087
C	1.163914	0.000000	2.192534
C	2.437499	-0.000466	1.591885
C	2.481354	-0.000451	0.189067
C	1.327176	-0.000113	-0.579668
N	-1.150256	0.000178	-0.672414
H	-0.969075	0.000265	1.937709
H	1.088562	0.000320	3.279568
H	3.344828	-0.000455	2.186858
H	3.447600	-0.000469	-0.315131
H	1.406487	0.000102	-1.666277
H	-0.942869	0.000482	-1.673993

4-CH3-PhNH(-) E=-326.414662 hartree

C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.445140
C	1.162900	0.000000	2.193482
C	2.446513	0.003766	1.609798
C	2.479482	0.008689	0.207006
C	1.328209	0.009297	-0.570031
N	-1.151093	-0.000968	-0.673391
H	-0.968448	0.004674	1.937870
H	1.081258	0.000303	3.281408
C	3.703006	-0.049902	2.444733
H	3.447643	0.015682	-0.296183
H	1.417653	0.022429	-1.655589
H	-0.942618	0.002283	-1.674668
H	4.578658	0.250598	1.857206
H	3.651958	0.622185	3.312498
H	3.919644	-1.055325	2.842159

4-OCH3-PhNH(-) $E=-401.641332$ hartree				4-OH-PhNH(-) $E=-362.331079$ hartree			
C	0.000000	0.000000	0.000000	C	0.000000	0.000000	0.000000
C	0.000000	0.000000	1.445630	C	0.000000	0.000000	1.445196
C	1.162982	0.000000	2.197137	C	1.163774	0.000000	2.197193
C	2.423788	-0.002613	1.585499	C	2.424133	-0.016157	1.586994
C	2.484921	-0.018734	0.190447	C	2.485085	-0.001254	0.194129
C	1.327416	-0.020222	-0.577690	C	1.327024	0.007397	-0.575756
N	-1.151803	0.009491	-0.672068	N	-1.152953	-0.002298	-0.671922
H	-0.967486	-0.006412	1.939205	H	-0.967311	0.011100	1.938974
H	1.107061	-0.011002	3.284002	H	1.107125	0.017021	3.284239
O	3.601862	-0.035186	2.359192	O	3.615073	0.011631	2.360785
H	3.460055	-0.043819	-0.292509	H	3.461155	0.006704	-0.286846
H	1.410556	-0.042934	-1.663090	H	1.412461	0.022584	-1.661100
H	-0.947000	0.002162	-1.673775	H	-0.946967	0.003466	-1.673392
C	4.084597	1.247940	2.714753	H	3.774044	-0.879407	2.686330
H	4.994009	1.102211	3.308157				
H	4.326893	1.847956	1.826160				
H	3.350367	1.804605	3.313902				

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