Table 1: Fully optimized quadruple-ζ valence basis sets for the *soft*-ECPs of Lester *et al.*

carbon		nitrogen	
exponent	contr. coefficient	exponent	contr. coefficient
4 s		3 s	
30.079038797	0.9307841321D-02	32.815496813	0.3737637272D-03
13.798991191	-0.5059941645D-01	9.8804259347	-0.1499609498D+00
4.0240229641	0.1955382686D+00	4.8763156756	0.1134757456D+01
2.9905908484	0.8372900664D+00	—	—
1 s		1 s	
0.67180242015	1.0000000000	0.85526831856	1.0000000000
1 s		1 s	
0.28163359813	1.0000000000	0.34982584055	1.0000000000
1 s		1 s	
0.11061937320	1.0000000000	0.14076282637	1.0000000000
3 p		3 p	
22.889787843	0.6707188470D-02	39.349383483	0.3769157396D-02
6.0344005729	0.2404188727D+00	8.5210899310	0.2463575530D+00
1.9889331346	0.8160425803D+00	2.9163634327	0.8089768435D+00
1 p		1 p	
0.71337962321	1.0000000000	1.0571098419	1.0000000000
1 p		1 p	
0.26185944096	1.0000000000	0.38553182845	1.0000000000
1 p		1 p	
0.94305432343E-01	1.0000000000	0.13527814998	1.0000000000

oxygen	
exponent	contr. coefficient
4 s	
29.559696738	-0.7238441963D-01
23.381964645	0.1433301911D+00
7.3384571970	-0.2489484449D+00
6.0388306641	-0.8095247133D+00
1 s	
1.1410682666	1.0000000000
1 s	
0.45063842512	1.0000000000
1 s	
0.17874408950	1.0000000000
3 p	
16.851192625	0.7279634196D-01
6.8592557909	0.2833861237D+00
2.5793361387	0.7292630406D+00
1 p	
0.99829032945	1.0000000000
1 p	
0.37900771321	1.0000000000
1 p	
0.13814070838	1.0000000000

Table 2: CGTOs obtained by least square fits to the respective STOs.

$\zeta = 1.0$		$\zeta = 0.82$	
exponent	contr. coefficient	exponent	contr. coefficient
10 s		10 s	
0.3624131448D+03	0.2023471024D-03	0.3052710500D+03	0.1619170226D-03
0.9617419337D+02	0.9179412159D-03	0.7544694241D+02	0.7945776495D-03
0.2963185085D+02	0.3586849412D-02	0.2209773935D+02	0.3279830431D-02
0.1014106805D+02	0.1238230590D-01	0.7285249035D+01	0.1178942969D-01
0.3764327203D+01	0.3810477779D-01	0.2630717471D+01	0.3732916748D-01
0.1491762029D+01	0.1027450710D+00	0.1023020226D+01	0.1023393771D+00
0.6240619606D+00	0.2285637971D+00	0.4233215353D+00	0.2290597803D+00
0.2731352232D+00	0.3652962688D+00	0.1843767675D+00	0.3662038268D+00
0.1237533501D+00	0.3148909407D+00	0.8340310389D-01	0.3155244675D+00
0.5642630518D-01	0.7822000665D-01	0.3800918848D-01	0.7843871491D-01

The respective exponents of the cusp-correction STOs were: 1.035 and 0.800. The correction radius was 0.1 a_0. See *J. Chem. Phys.* **115**, 5362 (2001) for the technical details of the cusp-correction.

Table 3: Fully optimized valence basis set for hydrogen (used for construction of the hydrogen aug-QZ basis set).

exponent	contr. coefficient
6 s	
0.3809822997D+03	0.1036581121D-02
0.9615989815D+02	0.3896287979D-02
0.2880216797D+02	0.1556761922D-01
0.1034717501D+02	0.5302524022D-01
0.3287800110D+01	0.2398156282D+00
0.1036766173D+01	0.7637865054D+00
1 s	
0.4425748951D+00	0.1000000000D+01
1 s	
0.2288624542D+00	0.1000000000D+01
1 s	
0.8927715045D-01	0.1000000000D+01

The exponent of the cusp-correction STO of the contracted basis function was 1.186. The correction radius was 0.1 a_0. See *J. Chem. Phys.* **115**, 5362 (2001) for the technical details of the cusp-correction.