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APPENDIX 1

Exponents and Coefficients of STO-3G basis set

Atom	Shell	Exponent	Coefficient		
C	S 3 1.00	.7161683735D+02	.1543289673D+00		
		.1304509632D+02	.5353281423D+00		
		.3530512160D+01	.4446345422D+00		
	SP 3 1.00	.2941249355D+01	-.9996722919D-01	.1559162750D+00	
		.6834830964D+00	.3995128261D+00	.6076837186D+00	
		.2222899159D+00	.7001154689D+00	.3919573931D+00	
Li	S 3 1.00	.1611957475D+02	.1543289673D+00		
		.2936200663D+01	.5353281423D+00		
		.7946504870D+00	.4446345422D+00		
	SP 3 1.00	.6362897469D+00	-.9996722919D-01	.1559162750D+00	
		.1478600533D+00	.3995128261D+00	.6076837186D+00	
		.4808867840D-01	.7001154689D+00	.3919573931D+00	

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Exponents and Coefficients of 6-31G basis set

Atom	Shell	Exponent	Coefficient	
C	S 6 1.00	.3047524880D+04	.1834737130D-02	
		.4573695180D+03	.1403732280D-01	
		.1039486850D+03	.6884262220D-01	
		.2921015530D+02	.2321844430D+00	
		.9286662960D+01	.4679413480D+00	
		.3163926960D+01	.3623119850D+00	
	SP 3 1.00	.7868272350D+01	-.1193324200D+00	.6899906660D-01
		.1881288540D+01	-.1608541520D+00	.3164239610D+00
		.5442492580D+00	.1143456440D+01	.7443082910D+00
	SP 1 1.00	.1687144782D+00	.1000000000D+01	.1000000000D+01
Li	S 6 1.00	.6424189150D+03	.2142607810D-02	
		.9679851530D+02	.1620887150D-01	
		.2209112120D+02	.7731557250D-01	
		.6201070250D+01	.2457860520D+00	
		.1935117680D+01	.4701890040D+00	
		.6367357890D+00	.3454708450D+00	
	SP 3 1.00	.2324918408D+01	-.3509174590D-01	.8941508040D-02
		.6324303556D+00	-.1912328440D+00	.1410094640D+00
		.7905343475D-01	.1083987800D+01	.9453636950D+00
	SP 1 1.00	.3596197175D-01	.1000000000D+01	.1000000000D+01

Exponents and Coefficients of DZP basis set

Atom	Shell	Exponent	Coefficient
C	S 3 1.00	.4232610000D+04	.2029000000D-02
		.6348820000D+03	.1553500000D-01
		.1460970000D+03	.7541099936D-01
		.4249740000D+02	.2571210000D+00
		.5965550000D+00	.1418920000D+02
		.1966600000D+01	.2425169945D+00
	S 1 1.00	.5147700000D+01	.1000000000D+01
	S 1 1.00	.4962000000D+00	.1000000000D+01
	S 1 1.00	.1533000000D+00	.1000000000D+01
	P 4 1.00	.1815570000D+02	.1853400000D-01
		.3986400000D+01	.1154420000D+00
		.1142900000D+01	.3862060000D+00
		.3594000000D+00	.6400890000D+00
	P 1 1.00	.1146000000D+00	.1000000000D+01
D 1 1.00	.7500000000D+00	.1000000000D+01	

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Atom	Shell	Exponent	Coefficient
Li	S 6 1.00	.9213000000D+03	.1367000000D-02
		.1387000000D+03	.1042500000D-01
		.3194000000D+02	.4985900000D-01
		.9353000000D+01	.1607010000D+00
		.3158000000D+01	.3446040000D+00
		.1157000000D+01	.4251970000D+00
	S 1 1.00	.4446000000D+00	.1694680000D+00
	S 1 1.00	.4446000000D+00	-.2223110000D+00
	S 1 1.00	.7666000000D-01	.1116477000D+01
	P 4 1.00	.2864000000D-01	.0000000000D+00
		.1488000000D+01	.3877000000D-01
		.2667000000D+00	.2362570000D+00
		.7201000000D-01	.8304480000D+00
	P 1 1.00	.2370000000D-01	.1000000000D+01
D 1 1.00	.2000000000D+00	.1000000000D+01	

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APPENDIX 2

Gaussian 92 input file

```
$RunGauss
%chk=12lic60
%nosave
%mem=6000000
# HF STO-3G opt scf=(direct,tight)
```

```
Optimize(start,C60+12Li)
```

```
0 13
C
C,1,R2
C,1,R3,2,A3
C,1,R4,2,A4,3,D4,0
C,2,R5,1,A5,3,D5,0
C,2,R6,1,A6,5,D6,0
C,3,R7,1,A7,2,D7,0
C,4,R8,1,A8,2,D8,0
C,3,R9,1,A9,7,D9,0
C,4,R10,1,A10,8,D10,0
C,7,R11,3,A11,1,D11,0
C,8,R12,4,A12,1,D12,0
C,9,R13,3,A13,1,D13,0
C,10,R14,4,A14,1,D14,0
C,5,R15,2,A15,1,D15,0
C,6,R16,2,A16,1,D16,0
C,5,R17,2,A17,15,D17,0
C,6,R18,2,A18,16,D18,0
C,11,R19,7,A19,3,D19,0
C,12,R20,8,A20,4,D20,0
C,13,R21,9,A21,3,D21,0
C,14,R22,10,A22,4,D22,0
C,15,R23,5,A23,2,D23,0
C,16,R24,6,A24,2,D24,0
C,17,R25,5,A25,2,D25,0
C,18,R26,6,A26,2,D26,0
C,11,R27,7,A27,19,D27,0
C,12,R28,8,A28,20,D28,0
C,19,R29,11,A29,7,D29,0
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C,20,R30,12,A30,8,D30,0
 C,25,R31,17,A31,5,D31,0
 C,26,R32,18,A32,6,D32,0
 C,21,R33,13,A33,9,D33,0
 C,22,R34,14,A34,10,D34,0
 C,23,R35,15,A35,5,D35,0
 C,27,R36,11,A36,7,D36,0
 C,24,R37,16,A37,6,D37,0
 C,28,R38,12,A38,8,D38,0
 C,29,R39,19,A39,11,D39,0
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 C,31,R43,25,A43,17,D43,0
 C,32,R44,26,A44,18,D44,0
 C,35,R45,23,A45,15,D45,0
 C,37,R46,24,A46,16,D46,0
 C,33,R47,21,A47,13,D47,0
 C,34,R48,22,A48,14,D48,0
 C,47,R49,33,A49,21,D49,0
 C,48,R50,34,A50,22,D50,0
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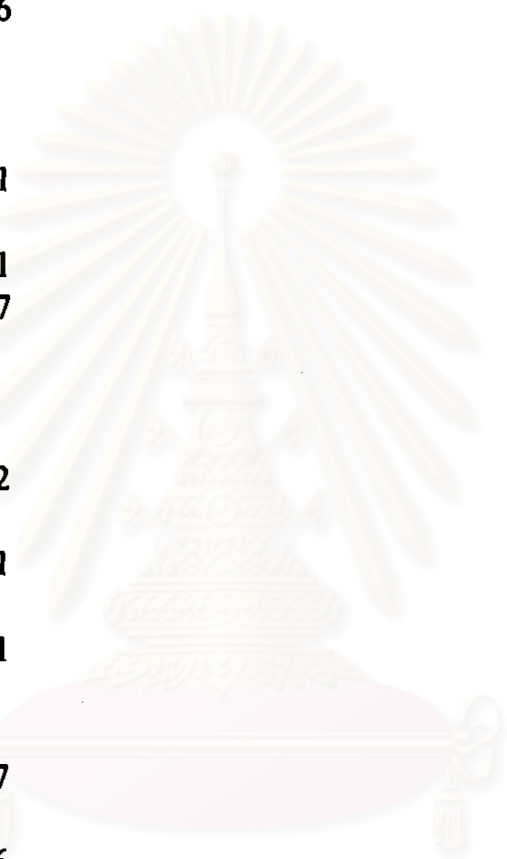
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D24=-138.1896567
D25=-142.62265172
D26=142.62261541
D27=-142.62262921
D28=142.62261541
D29=-142.62261541
D30=142.62262921
D31=138.1896567
D32=-138.18968117
D33=142.62261541
D34=-142.62264996
D35=-0.00002443
D36=138.1896567
D37=-0.00002445
D38=-138.18968117
D39=0.00002446
D40=138.18965671
D41=0.
D42=-138.18968117
D43=-142.622613
D44=142.62262921
D45=-138.1896567
D46=138.18974978
D47=-142.62262921
D48=142.622613



สำนักวิทยบริการ
มหาวิทยาลัย

D49=138.18968117
D50=-138.1896567
D51=142.62265172
D52=-142.622613
D53=-142.62262921
D54=142.62261541
D55=142.62264996
D56=-142.62261541
D57=-142.62261541
D58=142.62261541
D59=-142.62262921
D60=142.62262921
R61=1.2317
A61=54.0000
A62=90.0000
D61=0.00000
D62=90.00000



สถาบันวิทยบริการ
จุฬาลงกรณ์มหาวิทยาลัย

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