

## Supplementary Information (SI-1)

# Three-Body Excitations in Fock-Space Coupled-Cluster: Fourth Order Perturbation Correction to Electron Affinity and Its Relation to Bondonic Formalism

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A.1Di-Lithium Molecule ( $\text{Li}_2$ ): at internuclear distance 5.05 a.u

### Basis-A

li	3.0	0.0000	0.0000	0.0000
S	8			
1	1469.0000000	0.000765601232		
1	220.5000000	0.005888932715		
1	50.2600000	0.029655553732		
1	14.2400000	0.109123162563		
1	4.5810000	0.282641784375		
1	1.5800000	0.452887111102		
1	0.5640000	0.274630956861		
1	0.0734500	0.009745923779		
S	8			
2	1469.0000000	-0.000224991961		
2	220.5000000	-0.001730563167		
2	50.2600000	-0.008791560880		
2	14.2400000	-0.033152565467		
2	4.5810000	-0.091687974012		
2	1.5800000	-0.180010443274		

	2	0.5640000	-0.255703363785	
	2	0.0734500	1.078277723416	
S	1			
	3	0.0280500	1.000000000000	
P	3			
	4	1.5340000	0.038003981035	
	4	0.2749000	0.232032118583	
	4	0.0736200	0.834631408456	
P	1			
	5	0.0240300	1.000000000000	
D	1			
	6	0.1239000	1.000000000000	
li		3.0	0.0000	0.0000
				5.0512375652
S	8			
7	1469.0000000		0.000765601232	
	7	220.5000000	0.005888932715	
	7	50.2600000	0.02965553732	
	7	14.2400000	0.109123162563	
	7	4.5810000	0.282641784375	
	7	1.5800000	0.452887111102	
	7	0.5640000	0.274630956861	
	7	0.0734500	0.009745923779	
S	8			
8	1469.0000000		-0.000224991961	
	8	220.5000000	-0.001730563167	
	8	50.2600000	-0.008791560880	
	8	14.2400000	-0.033152565467	
	8	4.5810000	-0.091687974012	
	8	1.5800000	-0.180010443274	
	8	0.5640000	-0.255703363785	
	8	0.0734500	1.078277723416	
S	1			
	9	0.0280500	1.000000000000	
P	3			
	10	1.5340000	0.038003981035	
	10	0.2749000	0.232032118583	
	10	0.0736200	0.834631408456	
P	1			
	11	0.0240300	1.000000000000	
D	1			
	12	0.1239000	1.000000000000	

### Basis-B

li		3.0	0.0000	0.0000	0.0000
S	8				
1	1469.0000000		0.000765601232		
	1	220.5000000	0.005888932715		

1	50.2600000	0.029655553732
1	14.2400000	0.109123162563
1	4.5810000	0.282641784375
1	1.5800000	0.452887111102
1	0.5640000	0.274630956861
1	0.0734500	0.009745923779
S	8	
2	1469.0000000	-0.000224991961
2	220.5000000	-0.001730563167
2	50.2600000	-0.008791560880
2	14.2400000	-0.033152565467
2	4.5810000	-0.091687974012
2	1.5800000	-0.180010443274
2	0.5640000	-0.255703363785
2	0.0734500	1.078277723416
S	1	
3	0.0280500	1.000000000000
S	1	
4	0.0074000	1.000000000000
P	3	
5	1.5340000	0.038003981035
5	0.2749000	0.232032118583
5	0.0736200	0.834631408456
P	1	
6	0.0240300	1.000000000000
P	1	
7	0.0074000	1.000000000000
D	1	
8	0.1239000	1.000000000000
li	3.0	0.0000
		0.0000
		5.0512375652
S	8	
9	1469.0000000	0.000765601232
9	220.5000000	0.005888932715
9	50.2600000	0.029655553732
9	14.2400000	0.109123162563
9	4.5810000	0.282641784375
9	1.5800000	0.452887111102
9	0.5640000	0.274630956861
9	0.0734500	0.009745923779
S	8	
10	1469.0000000	-0.000224991961
10	220.5000000	-0.001730563167
10	50.2600000	-0.008791560880
10	14.2400000	-0.033152565467
10	4.5810000	-0.091687974012
10	1.5800000	-0.180010443274
10	0.5640000	-0.255703363785
10	0.0734500	1.078277723416
S	1	
11	0.0280500	1.000000000000

S	1		
	12	0.0074000	1.000000000000
P	3		
	13	1.5340000	0.038003981035
	13	0.2749000	0.232032118583
	13	0.0736200	0.834631408456
P	1		
	14	0.0240300	1.000000000000
P	1		
	15	0.0074000	1.000000000000
D	1		
	16	0.1239000	1.000000000000

### Basis-C

li	3.0	0.0000	0.0000	0.0000
S	9			
1	5988.0000000	0.000133195806		
	1 898.9000000	0.001026509035		
	1 205.9000000	0.005279761591		
	1 59.2400000	0.020959812281		
	1 19.8700000	0.066437667674		
	1 7.4060000	0.166019058768		
	1 2.9300000	0.315501808091		
	1 1.1890000	0.394102355987		
	1 0.4798000	0.191151004356		
S	9			
2	5988.0000000	-0.000077656259		
	2 898.9000000	-0.000595364655		
	2 205.9000000	-0.003032292029		
	2 59.2400000	-0.012299272305		
	2 19.8700000	-0.038898390070		
	2 7.4060000	-0.103900377014		
	2 2.9300000	-0.206846691413		
	2 1.1890000	-0.366970200153		
	2 0.4798000	-0.414865622550		
S	1			
	3	0.0750900	1.000000000000	
S	1			
	4	0.0283200	1.000000000000	
P	3			
	5	3.2660000	0.035544688557	
	5	0.6511000	0.195796454763	
	5	0.1696000	0.863995412271	
P	1			
	6	0.0557800	1.000000000000	
P	1			
	7	0.0205000	1.000000000000	
D	1			
	8	0.1239000	1.000000000000	

li	3.0	0.0000	0.0000	5.0512375652
S	9			
9	5988.0000000		0.000133195806	
9	898.9000000		0.001026509035	
9	205.9000000		0.005279761591	
9	59.2400000		0.020959812281	
9	19.8700000		0.066437667674	
9	7.4060000		0.166019058768	
9	2.9300000		0.315501808091	
9	1.1890000		0.394102355987	
9	0.4798000		0.191151004356	
S	9			
10	5988.0000000	-0.000077656259		
10	898.9000000	-0.000595364655		
10	205.9000000	-0.003032292029		
10	59.2400000	-0.012299272305		
10	19.8700000	-0.038898390070		
10	7.4060000	-0.103900377014		
10	2.9300000	-0.206846691413		
10	1.1890000	-0.366970200153		
10	0.4798000	-0.414865622550		
S	1			
11	0.0750900	1.000000000000		
S	1			
12	0.0283200	1.000000000000		
P	3			
13	3.2660000	0.035544688557		
13	0.6511000	0.195796454763		
13	0.1696000	0.863995412271		
P	1			
14	0.0557800	1.000000000000		
P	1			
15	0.0205000	1.000000000000		
D	1			
16	0.1239000	1.000000000000		

### Basis-D

li	3.0	0.0000	0.0000	0.0000
S	9			
1	5988.0000000	0.000133195806		
1	898.9000000	0.001026509035		
1	205.9000000	0.005279761591		
1	59.2400000	0.020959812281		
1	19.8700000	0.066437667674		
1	7.4060000	0.166019058768		
1	2.9300000	0.315501808091		
1	1.1890000	0.394102355987		
1	0.4798000	0.191151004356		

S	9			
2	5988.0000000		-0.000077656259	
2	898.9000000		-0.000595364655	
2	205.9000000		-0.003032292029	
2	59.2400000		-0.012299272305	
2	19.8700000		-0.038898390070	
2	7.4060000		-0.103900377014	
2	2.9300000		-0.206846691413	
2	1.1890000		-0.366970200153	
2	0.4798000		-0.414865622550	
S	1			
3	0.0750900		1.000000000000	
S	1			
4	0.0283200		1.000000000000	
S	1			
5	0.0074000		1.000000000000	
P	3			
6	3.2660000		0.035544688557	
6	0.6511000		0.195796454763	
6	0.1696000		0.863995412271	
P	1			
7	0.0557800		1.000000000000	
P	1			
8	0.0205000		1.000000000000	
P	1			
9	0.0074000		1.000000000000	
D	1			
10	0.1239000		1.000000000000	
li	3.0	0.0000	0.0000	5.0512375652
S	9			
11	5988.0000000		0.000133195806	
11	898.9000000		0.001026509035	
11	205.9000000		0.005279761591	
11	59.2400000		0.020959812281	
11	19.8700000		0.066437667674	
11	7.4060000		0.166019058768	
11	2.9300000		0.315501808091	
11	1.1890000		0.394102355987	
11	0.4798000		0.191151004356	
S	9			
12	5988.0000000		-0.000077656259	
12	898.9000000		-0.000595364655	
12	205.9000000		-0.003032292029	
12	59.2400000		-0.012299272305	
10	19.8700000		-0.038898390070	
10	7.4060000		-0.103900377014	
10	2.9300000		-0.206846691413	
12	1.1890000		-0.366970200153	
12	0.4798000		-0.414865622550	
S	1			

	13	0.0750900	1.000000000000
S	1		
	14	0.0283200	1.000000000000
S	1		
	15	0.0074000	1.000000000000
P	3		
	16	3.2660000	0.035544688557
	16	0.6511000	0.195796454763
	16	0.1696000	0.863995412271
P	1		
	17	0.0557800	1.000000000000
P	1		
	18	0.0205000	1.000000000000
P	1		
	19	0.0074000	1.000000000000
D	1		
	20	0.1239000	1.000000000000

## A.2 Di-Lithium Molecule ( $\text{Li}_2$ ): at internuclear distance 6.0 a.u

### Basis-A

li	3.0	0.0000	0.0000	0.0000
S	8			
1	1469.0000000	0.000765601232		
1	220.5000000	0.005888932715		
1	50.2600000	0.029655553732		
1	14.2400000	0.109123162563		
1	4.5810000	0.282641784375		
1	1.5800000	0.452887111102		
1	0.5640000	0.274630956861		
1	0.0734500	0.009745923779		
S	8			
2	1469.0000000	-0.000224991961		
2	220.5000000	-0.001730563167		
2	50.2600000	-0.008791560880		
2	14.2400000	-0.033152565467		
2	4.5810000	-0.091687974012		
2	1.5800000	-0.180010443274		
2	0.5640000	-0.255703363785		
2	0.0734500	1.078277723416		
S	1			
3	0.0280500	1.000000000000		
P	3			

	4	1.5340000	0.038003981035	
	4	0.2749000	0.232032118583	
	4	0.0736200	0.834631408456	
P	1			
	5	0.0240300	1.000000000000	
D	1			
	6	0.1239000	1.000000000000	
li	3.0	0.0000	0.0000	6.0000
S	8			
7	1469.0000000	0.000765601232		
	7	220.5000000	0.005888932715	
	7	50.2600000	0.02965553732	
	7	14.2400000	0.109123162563	
	7	4.5810000	0.282641784375	
	7	1.5800000	0.452887111102	
	7	0.5640000	0.274630956861	
	7	0.0734500	0.009745923779	
S	8			
8	1469.0000000	-0.000224991961		
	8	220.5000000	-0.001730563167	
	8	50.2600000	-0.008791560880	
	8	14.2400000	-0.033152565467	
	8	4.5810000	-0.091687974012	
	8	1.5800000	-0.180010443274	
	8	0.5640000	-0.255703363785	
	8	0.0734500	1.078277723416	
S	1			
	9	0.0280500	1.000000000000	
P	3			
	10	1.5340000	0.038003981035	
	10	0.2749000	0.232032118583	
	10	0.0736200	0.834631408456	
P	1			
	11	0.0240300	1.000000000000	
D	1			
	12	0.1239000	1.000000000000	

### Basis-B

li	3.0	0.0000	0.0000	0.0000
S	8			
1	1469.0000000	0.000765601232		
	1	220.5000000	0.005888932715	
	1	50.2600000	0.02965553732	
	1	14.2400000	0.109123162563	
	1	4.5810000	0.282641784375	
	1	1.5800000	0.452887111102	
	1	0.5640000	0.274630956861	
	1	0.0734500	0.009745923779	



S	8			
2	1469.0000000		-0.000224991961	
	2	220.5000000	-0.001730563167	
	2	50.2600000	-0.008791560880	
	2	14.2400000	-0.033152565467	
	2	4.5810000	-0.091687974012	
	2	1.5800000	-0.180010443274	
	2	0.5640000	-0.255703363785	
	2	0.0734500	1.078277723416	
S	1			
	3	0.0280500	1.000000000000	
S	1			
	4	0.0074000	1.000000000000	
P	3			
	5	1.5340000	0.038003981035	
	5	0.2749000	0.232032118583	
	5	0.0736200	0.834631408456	
P	1			
	6	0.0240300	1.000000000000	
P	1			
	7	0.0074000	1.000000000000	
D	1			
	8	0.1239000	1.000000000000	
li	3.0	0.0000	0.0000	6.0000
S	8			
9	1469.0000000		0.000765601232	
	9	220.5000000	0.005888932715	
	9	50.2600000	0.029655553732	
	9	14.2400000	0.109123162563	
	9	4.5810000	0.282641784375	
	9	1.5800000	0.452887111102	
	9	0.5640000	0.274630956861	
	9	0.0734500	0.009745923779	
S	8			
10	1469.0000000		-0.000224991961	
	10	220.5000000	-0.001730563167	
	10	50.2600000	-0.008791560880	
	10	14.2400000	-0.033152565467	
	10	4.5810000	-0.091687974012	
	10	1.5800000	-0.180010443274	
	10	0.5640000	-0.255703363785	
	10	0.0734500	1.078277723416	
S	1			
	11	0.0280500	1.000000000000	
S	1			
	12	0.0074000	1.000000000000	
P	3			
	13	1.5340000	0.038003981035	
	13	0.2749000	0.232032118583	
	13	0.0736200	0.834631408456	

P	1		
	14	0.0240300	1.00000000000000
P	1		
	15	0.0074000	1.00000000000000
D	1		
	16	0.1239000	1.00000000000000

# Basis-C

li	3.0	0.0000	0.0000	0.0000
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S	9		
1	5988.0000000	0.000133195806	
1	898.9000000	0.001026509035	
1	205.9000000	0.005279761591	
1	59.2400000	0.020959812281	
1	19.8700000	0.066437667674	
1	7.4060000	0.166019058768	
1	2.9300000	0.315501808091	
1	1.1890000	0.394102355987	
1	0.4798000	0.191151004356	

S	9		
2	5988.0000000	-0.000077656259	
2	898.9000000	-0.000595364655	
2	205.9000000	-0.003032292029	
2	59.2400000	-0.012299272305	
2	19.8700000	-0.038898390070	
2	7.4060000	-0.103900377014	
2	2.9300000	-0.206846691413	
2	1.1890000	-0.366970200153	
2	0.4798000	-0.414865622550	

S	1		
3	0.0750900	1.00000000000000	

S	1		
4	0.0283200	1.00000000000000	

P	3		
5	3.2660000	0.035544688557	
5	0.6511000	0.195796454763	
5	0.1696000	0.863995412271	

P	1		
6	0.0557800	1.00000000000000	

P	1		
7	0.0205000	1.00000000000000	

D	1		
8	0.1239000	1.00000000000000	

li	3.0	0.0000	0.0000	6.0000
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S	9		
9	5988.0000000	0.000133195806	
9	898.9000000	0.001026509035	
9	205.9000000	0.005279761591	

9	59.2400000	0.020959812281
9	19.8700000	0.066437667674
9	7.4060000	0.166019058768
9	2.9300000	0.315501808091
9	1.1890000	0.394102355987
9	0.4798000	0.191151004356
S	9	
10	5988.0000000	-0.000077656259
10	898.9000000	-0.000595364655
10	205.9000000	-0.003032292029
10	59.2400000	-0.012299272305
10	19.8700000	-0.038898390070
10	7.4060000	-0.103900377014
10	2.9300000	-0.206846691413
10	1.1890000	-0.366970200153
10	0.4798000	-0.414865622550
S	1	
11	0.0750900	1.000000000000
S	1	
12	0.0283200	1.000000000000
P	3	
13	3.2660000	0.035544688557
13	0.6511000	0.195796454763
13	0.1696000	0.863995412271
P	1	
14	0.0557800	1.000000000000
P	1	
15	0.0205000	1.000000000000
D	1	
16	0.1239000	1.000000000000

# Basis-D

li	3.0	0.0000	0.0000	0.0000
S	9			
1	5988.0000000	0.000133195806		
1	898.9000000	0.001026509035		
1	205.9000000	0.005279761591		
1	59.2400000	0.020959812281		
1	19.8700000	0.066437667674		
1	7.4060000	0.166019058768		
1	2.9300000	0.315501808091		
1	1.1890000	0.394102355987		
1	0.4798000	0.191151004356		
S	9			
2	5988.0000000	-0.000077656259		
2	898.9000000	-0.000595364655		
2	205.9000000	-0.003032292029		
2	59.2400000	-0.012299272305		
2	19.8700000	-0.038898390070		

	2	7.4060000	-0.103900377014	
	2	2.9300000	-0.206846691413	
	2	1.1890000	-0.366970200153	
	2	0.4798000	-0.414865622550	
S	1			
	3	0.0750900	1.000000000000	
S	1			
	4	0.0283200	1.000000000000	
S	1			
	5	0.0074000	1.000000000000	
P	3			
	6	3.2660000	0.035544688557	
	6	0.6511000	0.195796454763	
	6	0.1696000	0.863995412271	
P	1			
	7	0.0557800	1.000000000000	
P	1			
	8	0.0205000	1.000000000000	
P	1			
	9	0.0074000	1.000000000000	
D	1			
	10	0.1239000	1.000000000000	
li		3.0	0.0000	0.0000
S	9			6.0000
	11	5988.0000000	0.000133195806	
	11	898.9000000	0.001026509035	
	11	205.9000000	0.005279761591	
	11	59.2400000	0.020959812281	
	11	19.8700000	0.066437667674	
	11	7.4060000	0.166019058768	
	11	2.9300000	0.315501808091	
	11	1.1890000	0.394102355987	
	11	0.4798000	0.191151004356	
S	9			
12		5988.0000000	-0.000077656259	
	12	898.9000000	-0.000595364655	
	12	205.9000000	-0.003032292029	
	12	59.2400000	-0.012299272305	
	10	19.8700000	-0.038898390070	
	10	7.4060000	-0.103900377014	
	10	2.9300000	-0.206846691413	
	12	1.1890000	-0.366970200153	
	12	0.4798000	-0.414865622550	
S	1			
	13	0.0750900	1.000000000000	
S	1			
	14	0.0283200	1.000000000000	
S	1			
	15	0.0074000	1.000000000000	
P	3			

	16	3.2660000	0.035544688557
	16	0.6511000	0.195796454763
	16	0.1696000	0.863995412271
P	1		
	17	0.0557800	1.000000000000
P	1		
	18	0.0205000	1.000000000000
P	1		
	19	0.0074000	1.000000000000
D	1		
	20	0.1239000	1.000000000000