

**A Joint Experimental and Theoretical Study of Cation- $\pi$  Interactions:  
Multiple-Decker Sandwich Complexes of Ferrocene with Alkali Metal  
Ions ( $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Rb}^+$ ,  $\text{Cs}^+$ ).**

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**Supplementary Material**

**Theoretical Structures**

The coordinates of the theoretically calculated structures discussed along the manuscript together with the electronic energies are collected below.

### 3M

#### 3Li

B3LYP/TZ, E=-239.6733404

C	0.	0.121407729	1.3989191825
C	1.2114995499	0.121407729	0.6994595913
C	1.2114995499	0.121407729	-0.6994595913
C	0.	0.121407729	-1.3989191825
C	-1.2114995499	0.121407729	-0.6994595913
C	-1.2114995499	0.121407729	0.6994595913
H	2.1478766505	0.131445341	-1.2400771623
H	0.	0.131445341	-2.4801543247
H	-2.1478766505	0.131445341	-1.2400771623
H	-2.1478766505	0.131445341	1.2400771623
H	0.	0.131445341	2.4801543247
H	2.1478766505	0.131445341	1.2400771623
Li	0.	-1.7197834295	0.

#### 3Rb

B3LYP/DZ E=-255.9874223

C	0.000000	0.000000	1.402082
C	1.214239	0.000000	0.701041
C	1.214239	0.000000	-0.701041
C	0.000000	0.000000	-1.402082
C	-1.214239	0.000000	-0.701041
C	-1.214239	0.000000	0.701041
H	2.155200	0.000000	-1.244305
H	0.000000	0.000000	-2.488610
H	-2.155200	0.000000	-1.244305
H	-2.155200	0.000000	1.244305
H	0.000000	0.000000	2.488610
H	2.155200	0.000000	1.244305
Rb	0.000000	-3.275813	0.000000

# Ferrocene

B3LYP/TZ E=-1650.974346

Fe	0.	-0.0004044004	0
C	0.	1.2105163889	1.6888954779
H	-0.0000000001	2.2875645932	1.6745458745
C	1.1511518132	0.3741850295	1.6893790502
H	2.1752789198	0.7075123819	1.6755299767
C	.7114633625	-0.9791417964	1.6901381441
H	1.3446578031	-1.850474639	1.6777934084
C	-0.7114633618	-0.9791417967	1.6901381443
H	-1.3446578021	-1.8504746394	1.6777934087
C	-1.1511518129	0.3741850291	1.6893790505
H	-2.1752789196	0.7075123812	1.6755299773
C	-0.0000000004	1.2105163889	-1.6888954779
H	-0.0000000006	2.2875645932	-1.6745458745
C	1.1511518128	.3741850295	-1.6893790505
H	2.1752789193	.7075123819	-1.6755299773
C	.7114633621	-0.9791417964	-1.6901381443
H	1.3446578027	-1.850474639	-1.6777934087
C	-0.7114633622	-0.9791417967	-1.6901381441
H	-1.3446578025	-1.8504746394	-1.6777934084
C	-1.1511518133	.3741850291	-1.6893790502
H	-2.17527892	.7075123812	-1.6755299767

## 5M

### 5Li

B3LYP/TZ E= -1658.334285

C	0.	1.2228116671	-1.5719704331
C	1.1629630042	0.3778695861	-1.5719704331
C	0.7187506643	-0.9892754196	-1.5719704331
C	-0.7187506643	-0.9892754196	-1.5719704331
C	-1.1629630042	0.3778695861	-1.5719704331
C	0.	1.2090725084	1.791825133
C	1.1498962878	0.3736239525	1.791825133
C	0.7106749894	-0.9781602068	1.791825133
C	-0.7106749894	-0.9781602068	1.791825133
C	-1.1498962878	0.3736239525	1.791825133
Fe	0.	0.	0.09716621
H	0.	2.2998309244	-1.5578038123
Li	0.	0.	-3.4095081705
H	2.187269187	0.7106868398	-1.5578038123
H	1.3518067001	-1.860602302	-1.5578038123
H	-1.3518067001	-1.860602302	-1.5578038123
H	-2.187269187	0.7106868398	-1.5578038123
H	0.	2.2861823268	1.7791162228
H	2.1742885993	0.7064691912	1.7791162228
H	1.3437842557	-1.8495603546	1.7791162228
H	-1.3437842557	-1.8495603546	1.7791162228
H	-2.1742885993	0.7064691912	1.7791162228

**5Na**

B3LYP/TZ E=-1813.1104258

C	0.7174624512	-0.9875023465	-1.2642553773
C	1.1608786317	0.3771923324	-1.2642553773
C	0.	1.2206200282	-1.2642553773
C	-1.1608786317	0.3771923324	-1.2642553773
C	-0.7174624512	-0.9875023465	-1.2642553773
Fe	0.	0.	0.4016378738
C	0.7107405921	-0.9782505012	2.0983080733
C	1.1500024353	0.3736584419	2.0983080733
C	0.	1.2091841185	2.0983080733
C	-1.1500024353	0.3736584419	2.0983080733
C	-0.7107405921	-0.9782505012	2.0983080733
Na	0.	0.	-3.6137603168
H	0.	2.2974381346	-1.2301052042
H	-2.1849935087	0.7099474271	-1.2301052042
H	-1.3504002535	-1.8586664944	-1.2301052042
H	1.3504002535	-1.8586664944	-1.2301052042
H	2.1849935087	0.7099474271	-1.2301052042
H	0.	2.2861203754	2.0875447815
H	-2.1742296801	0.7064500472	2.0875447815
H	-1.3437478417	-1.8495102349	2.0875447815
H	1.3437478417	-1.8495102349	2.0875447815
H	2.1742296801	0.7064500472	2.0875447815

**5K**

B3LYP/TZ E=-2250.7688267

C	0.7159351876	-0.9854002484	-0.9422885354
C	1.1584074673	0.3763894024	-0.9422885354
C	0.	1.2180216921	-0.9422885354
C	-1.1584074673	0.3763894024	-0.9422885354
C	-0.7159351876	-0.9854002484	-0.9422885354
Fe	0.	0.	0.7319404319
C	0.7107903834	-0.978319033	2.4279362025
C	1.1500829993	0.3736846188	2.4279362025
C	0.	1.2092688285	2.4279362025
C	-1.1500829993	0.3736846188	2.4279362025
C	-0.7107903834	-0.978319033	2.4279362025
K	0.	0.	-3.7451092652
H	0.	2.2947064696	-0.9046547579
H	-2.1823955409	0.7091032962	-0.9046547579
H	-1.3487946211	-1.856456531	-0.9046547579
H	1.3487946211	-1.856456531	-0.9046547579
H	2.1823955409	0.7091032962	-0.9046547579
H	0.	2.2862671225	2.4160937169
H	-2.1743692449	0.7064953945	2.4160937169
H	-1.3438340974	-1.8496289558	2.4160937169
H	1.3438340974	-1.8496289558	2.4160937169
H	2.1743692449	0.7064953945	2.4160937169

**5Rb**

B3LYP/DZ E=-1674.3736634

C	-1.1625363697	0.3777309641	0.3260276978
C	1.1625363697	0.3777309641	0.3260276978
C	-1.155355904	0.3753978894	-3.02965866
C	1.155355904	0.3753978894	-3.02965866
C	0.	1.2223630771	0.3260276978
C	0.7184869896	-0.9889125026	0.3260276978
C	-0.7184869896	-0.9889125026	0.3260276978
C	-0.7140492178	-0.9828044336	-3.02965866
C	0.7140492178	-0.9828044336	-3.02965866
C	0.	1.2148130886	-3.02965866
Fe	0.	0.	-1.3421910988
Rb	0.	0.	3.5043675173
H	0.	2.3039981864	0.28382415
H	0.	2.296393424	-3.0149642916
H	1.3542561553	-1.8639736878	0.28382415
H	-1.3542561553	-1.8639736878	0.28382415
H	1.3497861881	-1.8578213058	-3.0149642916
H	-1.3497861881	-1.8578213058	-3.0149642916
H	-2.1912324887	0.7119745946	0.28382415
H	2.1839999298	0.7096245938	-3.0149642916
H	-2.1839999298	0.7096245938	-3.0149642916
H	2.1912324887	0.7119745946	0.28382415

## 6M<sub>2</sub>

### 6Li<sub>2</sub>

B3LYP/TZ E =-1665.5798695

Fe	0.	0.	0.
C	0.	1.2199192729	1.6847068145
H	0.	2.2978380105	1.6672733615
Li	0.	0.	3.6559615381
C	-1.1602121738	0.3769757871	1.6847068145
C	-0.7170505576	-0.9869354235	1.6847068145
C	0.7170505576	-0.9869354235	1.6847068145
C	1.1602121738	0.3769757871	1.6847068145
C	0.	1.2199192729	-1.6847068145
C	-1.1602121738	0.3769757871	-1.6847068145
C	-0.7170505576	-0.9869354235	-1.6847068145
C	0.7170505576	-0.9869354235	-1.6847068145
C	1.1602121738	0.3769757871	-1.6847068145
H	-2.1853738133	0.7100709956	1.6672733615
H	-1.3506352947	-1.8589900008	1.6672733615
H	1.3506352947	-1.8589900008	1.6672733615
H	2.1853738133	0.7100709956	1.6672733615
H	0.	2.2978380105	-1.6672733615
H	-2.1853738133	0.7100709956	-1.6672733615
H	-1.3506352947	-1.8589900008	-1.6672733615
H	1.3506352947	-1.8589900008	-1.6672733615
H	2.1853738133	0.7100709956	-1.6672733615
Li	0.	0.	-3.6559615381



**6Na<sub>2</sub>**

B3LYP/TZ E=-1975.1540935

Fe	0.	0.	0.
C	0.	1.217568806	1.6844082982
H	0.	2.2950192513	1.6535146269
Na	0.	0.	4.202590758
C	-1.157976747	0.3762494529	1.6844082982
C	-0.7156689878	-0.9850338559	1.6844082982
C	0.7156689878	-0.9850338559	1.6844082982
C	1.157976747	0.3762494529	1.6844082982
C	0.	1.217568806	-1.6844082982
C	-1.157976747	0.3762494529	-1.6844082982
C	-0.7156689878	-0.9850338559	-1.6844082982
C	0.7156689878	-0.9850338559	-1.6844082982
C	1.157976747	0.3762494529	-1.6844082982
H	-2.182693014	0.7091999511	1.6535146269
H	-1.3489784696	-1.8567095767	1.6535146269
H	1.3489784696	-1.8567095767	1.6535146269
H	2.182693014	0.7091999511	1.6535146269
H	0.	2.2950192513	-1.6535146269
H	-2.182693014	0.7091999511	-1.6535146269
H	-1.3489784696	-1.8567095767	-1.6535146269
H	1.3489784696	-1.8567095767	-1.6535146269
H	2.182693014	0.7091999511	-1.6535146269
Na	0.	0.	-4.202590758

**6K<sub>2</sub>**

B3LYP/TZ E= -2850.4842104

Fe	0.	0.	0.
C	0.	1.2151993173	1.6870509648
H	0.	2.2925120343	1.6536411846
K	0.	0.	4.7167716845
C	-1.1557232293	0.3755172406	1.6870509648
C	-0.7142762373	-0.9831168992	1.6870509648
C	0.7142762373	-0.9831168992	1.6870509648
C	1.1557232293	0.3755172406	1.6870509648
C	0.	1.2151993173	-1.6870509648
C	-1.1557232293	0.3755172406	-1.6870509648
C	-0.7142762373	-0.9831168992	-1.6870509648
C	0.7142762373	-0.9831168992	-1.6870509648
C	1.1557232293	0.3755172406	-1.6870509648
H	-2.1803085089	0.7084251784	1.6536411846
H	-1.3475047645	-1.8546811956	1.6536411846
H	1.3475047645	-1.8546811956	1.6536411846
H	2.1803085089	0.7084251784	1.6536411846
H	0.	2.2925120343	-1.6536411846
H	-2.1803085089	0.7084251784	-1.6536411846
H	-1.3475047645	-1.8546811956	-1.6536411846
H	1.3475047645	-1.8546811956	-1.6536411846
H	2.1803085089	0.7084251784	-1.6536411846
K	0.	0.	-4.7167716845

**6Rb<sub>2</sub>**

B3LYP/DZ E= -1698.0352516

Fe	0.	0.	0.
C	0.	1.219645329	1.6798642471
H	0.	2.3013882409	1.6406567662
Rb	0.	0.	5.1581223277
C	-1.1599516377	0.3768911338	1.6798642471
C	-0.7168895374	-0.9867137983	1.6798642471
C	0.7168895374	-0.9867137983	1.6798642471
C	1.1599516377	0.3768911338	1.6798642471
C	0.	1.219645329	-1.6798642471
C	-1.1599516377	0.3768911338	-1.6798642471
C	-0.7168895374	-0.9867137983	-1.6798642471
C	0.7168895374	-0.9867137983	-1.6798642471
C	1.1599516377	0.3768911338	-1.6798642471
H	-2.188750283	0.7111680771	1.6406567662
H	-1.3527220678	-1.8618621975	1.6406567662
H	1.3527220678	-1.8618621975	1.6406567662
H	2.188750283	0.7111680771	1.6406567662
H	0.	2.3013882409	-1.6406567662
H	-2.188750283	0.7111680771	-1.6406567662
H	-1.3527220678	-1.8618621975	-1.6406567662
H	1.3527220678	-1.8618621975	-1.6406567662
H	2.188750283	0.7111680771	-1.6406567662
Rb	0.	0.	-5.1581223277

## 7M

### 7Li

B3LYP/DZ E=-3308.8482765

Fe	0.0000000099	-0.0010405913	3.6500074515
C	-0.0000000978	1.2203171693	1.994769133
C	0.0000001125	1.2185209153	5.3267096549
C	0.7198069971	-0.9950609122	1.9986494734
C	-0.7198071679	-0.9950609198	1.9986495531
C	-1.1646943403	0.3741136533	1.9963643562
C	-1.1547425986	0.3796147515	5.3295520748
C	-0.7137055536	-0.9778906008	5.3341208558
C	0.713705813	-0.9778905899	5.3341207629
C	1.1547428358	0.3796147693	5.3295519204
C	1.1646941554	0.3741136667	1.9963642344
H	2.1840149108	0.7145927293	5.3084896355
H	2.1937083644	0.7091690908	2.0160922081
H	0.0000001033	2.3009070373	5.3027992385
H	-0.0000001027	2.3025784019	2.0138914444
H	1.3558822239	-1.8706484941	2.0195581494
H	1.349990828	-1.8537174955	5.3179437517
H	-1.3558823818	-1.8706485097	2.0195582848
H	-1.3499905547	-1.8537175179	5.3179439318
H	-2.1937085505	0.7091690664	2.0160924412
H	-2.1840146811	0.7145926965	5.3084899307
Li	-0.0000001379	-0.0032566298	0.000000061
C	-0.0000001439	1.2203171617	-1.9947690718
C	0.0000001361	1.2185209169	-5.3267097305
C	-1.1646943857	0.3741136604	-1.9963643725
C	-1.1547425836	0.379614772	-5.329552129
C	-0.7198072303	-0.9950609084	-1.9986495643
C	-0.7137055625	-0.9778905865	-5.3341208958
Fe	0.0000000399	-0.0010405721	-3.6500075209
C	0.7137058012	-0.9778906015	-5.3341208042
C	0.719806926	-0.9950609203	-1.9986494093
C	1.1547428402	0.3796147487	-5.3295519848
C	1.164694089	0.3741136476	-1.9963641026
H	-0.0000001343	2.302578395	-2.0138913558

Fe	0.0000000099	-0.0010405913	3.6500074515
H	0.000000148	2.3009070385	-5.3027993254
H	-1.355882459	-1.870648487	-2.0195583335
H	-1.3499905829	-1.8537174894	-5.317943934
H	1.3499908018	-1.8537175141	-5.3179437493
H	1.3558821455	-1.8706485084	-2.0195580575
H	2.1840149209	0.7145926927	-5.3084897178
H	2.1937083025	0.7091690627	-2.0160920225
H	-2.1840146624	0.7145927275	-5.3084899665
H	-2.1937085939	0.709169077	-2.0160924993

**7Na**

B3LYP/DZ E= -3463.6109277

Fe	-0.000000001	-0.0009037686	4.0812207854
C	-0.0000000021	1.2191027698	2.4246198514
C	-0.0000000006	1.2191709759	5.7576925347
C	0.7194494816	-0.9951362655	2.4296147853
C	-0.7194494852	-0.9951362657	2.4296147872
C	-1.1640835285	0.373370816	2.4265284213
C	-1.1547750927	0.3802460359	5.7607432979
C	-0.7137279792	-0.977323247	5.7656803107
C	0.7137279795	-0.9773232471	5.7656803129
C	1.1547750918	0.3802460362	5.7607432971
C	1.1640835246	0.3733708165	2.426528419
H	2.1840785409	0.7151359378	5.7402655711
H	2.1931970155	0.7083758404	2.4622251557
H	-0.0000000008	2.301561502	5.734191573
H	-0.0000000021	2.3014428691	2.4593546141
H	1.3557208972	-1.8706193172	2.467112023
H	1.3500338996	-1.8531445524	5.7500542425
H	-1.3557209005	-1.8706193168	2.4671120454
H	-1.3500338989	-1.8531445525	5.7500542372
H	-2.1931970192	0.7083758398	2.4622251629
H	-2.184078542	0.7151359368	5.7402655713
Na	0.0000000022	-0.0043697183	0.0000000056
C	0.0000000017	1.2191027739	-2.4246198458
C	0.0000000012	1.2191709749	-5.7576925378
C	-1.1640835245	0.3733708195	-2.4265284102
C	-1.1547750918	0.3802460366	-5.7607433002
C	-0.71944948	-0.995136262	-2.429614773
C	-0.7137279812	-0.9773232469	-5.7656803154
Fe	0.0000000002	-0.0009037685	-4.0812207871
C	0.7137279773	-0.9773232483	-5.7656803143
C	0.7194494873	-0.9951362614	-2.4296147764
C	1.1547750919	0.3802460337	-5.760743301
C	1.1640835291	0.373370821	-2.4265284124
H	-0.0000000012	2.301442873	-2.459354621
H	0.0000000032	2.301561501	-5.7341915768

Fe	-0.0000000001	-0.0009037686	4.0812207854
H	-1.355720894	-1.8706193143	-2.4671120342
H	-1.3500339025	-1.8531445513	-5.7500542418
H	1.3500338966	-1.8531445541	-5.7500542457
H	1.3557209026	-1.8706193123	-2.4671120264
H	2.1840785414	0.7151359339	-5.7402655768
H	2.1931970187	0.7083758455	-2.4622251798
H	-2.1840785406	0.7151359395	-5.7402655742
H	-2.1931970164	0.7083758409	-2.4622251544

**7K**

B3LYP/DZ E=-2850.0796527

Fe	0.0000106342	-0.0007165266	4.5623196004
C	-0.0001920058	1.2201244754	2.9015863054
C	0.0001992686	1.2161178958	6.2407489179
C	0.7181152473	-0.9905481727	2.902808162
C	-0.7185000148	-0.9905457151	2.9029716581
C	-1.1623853261	0.3757561686	2.9022521694
C	-1.1546682051	0.3771255739	6.2422696332
C	-0.7135836581	-0.98056096	6.2444688259
C	0.7139853282	-0.9805607361	6.2443067862
C	1.1550682518	0.3771265177	6.242010386
C	1.1620041086	0.3757564499	2.9019903177
H	2.1843551545	0.7120749586	6.2216700092
H	2.1913074949	0.7108215751	2.9433682356
H	0.0001960913	2.2985485764	6.2189592318
H	-0.0001821783	2.3026440198	2.9428160624
H	1.3545321927	-1.8662657638	2.9440681563
H	1.3502996584	-1.8563412964	6.2264183215
H	-1.3549029482	-1.8662661588	2.9443758838
H	-1.3499010937	-1.8563421004	6.2267231055
H	-2.1916779598	0.7108242097	2.9438607364
H	-2.1839598407	0.7120729661	6.22215835
K	-0.0002415914	-0.0016906091	-0.0000000203
C	-0.0001917797	1.2201243033	-2.9015862796
C	0.0001994252	1.2161179375	-6.2407488246
C	-1.1623851519	0.3757560711	-2.9022521615
C	-1.1546681804	0.3771257914	-6.2422694677
C	-0.7184999233	-0.9905458398	-2.9029717204
C	-0.713583838	-0.980560803	-6.2444688256
Fe	0.0000107263	-0.0007166072	-4.5623196618
C	0.7139851567	-0.9805608118	-6.2443069141
C	0.7181153376	-0.9905483889	-2.9028082563
C	1.1550682899	0.377126388	-6.2420104268
C	1.1620042848	0.3757562091	-2.9019903542
H	-0.000181886	2.3026438412	-2.9428159068



Fe	0.0000106342	-0.0007165266	4.5623196004
H	0.0001964136	2.2985486166	-6.218959032
H	-1.3549029046	-1.8662662474	-2.9443759673
H	-1.3499014148	-1.8563418293	-6.2267230454
H	1.3502992283	-1.8563414714	-6.2264186527
H	1.3545322277	-1.8662660178	-2.9440682837
H	2.1843552118	0.712074731	-6.2216701685
H	2.1913076934	0.7108212846	-2.9433682534
H	-2.183959759	0.7120733197	-6.2221579183
H	-2.191677766	0.7108241747	-2.9438607138

**8Li**

B3LYP/DZ E=-1867.5304282

C	3.1473304855	0.1260984134	-0.8823173916
C	3.1427731804	-0.8833791262	0.1279286858
C	2.7793596097	-0.2690661934	1.3648687114
C	2.5598496076	1.1205536567	1.118877388
C	2.7868809356	1.3648920321	-0.2698352916
Fe	1.2574766838	-0.0228158916	-0.0302433076
C	-0.0804582086	-0.5065504393	-1.5337399534
C	-0.0846619505	-1.5220928611	-0.5172146551
C	-0.4475026084	-0.9062166002	0.7259529443
C	-0.6780045741	0.4911855917	0.4768563799
C	-0.4438512505	0.7360308698	-0.9224666506
Li	-3.1684986164	0.2125096846	0.1228093355
H	0.1926733928	-2.5594910692	-0.6530330717
H	-0.5102141113	-1.4001536043	1.6860759612
H	-0.8946593162	1.2410949074	1.2283996206
H	-0.4917502847	1.6960092132	-1.4192593158
H	0.1856290948	-0.6482716598	-2.5727771775
H	3.3575948042	-1.932883786	-0.0217430876
H	2.6727844144	-0.7711151989	2.3169727462
H	2.25675834	1.8555926135	1.8523219614
H	2.687266611	2.3173752837	-0.7726509975
H	3.3671928131	-0.0249433287	-1.9305544453
O	-3.9449301048	-0.4255407067	1.791069907
N	-3.9668764849	1.991640775	-0.5247854882
O	-3.2353394158	-1.3795201137	-0.970968267
H	-4.0910281784	-1.3765853139	1.8848895443
H	-4.2209268982	-0.0161664437	2.6209036505
H	-3.8499716659	-1.7253639852	-1.6299835261
H	-2.345131107	-1.6899847509	-1.2090416725
H	-4.9802575747	2.0168799276	-0.41258361
H	-3.6139118662	2.8235933178	-0.0526890348
H	-3.7909461978	2.1403670827	-1.5181252581

**9Li**

B3LYP/DZ E=-2218.332751

C	-3.689327919	-0.2775278958	1.5754581837
C	-4.2251976795	-1.0905848196	0.5295112258
C	-4.4229885128	-0.2596984207	-0.6163750814
C	-4.0097552266	1.0658210335	-0.2760606904
C	-3.555459193	1.0545396899	1.0771736891
Fe	-2.4261096633	-0.2473297531	-0.063547717
C	-0.5656598174	-0.843828544	0.5688869526
C	-0.4724638943	0.4913282544	0.0147885896
C	-0.9292316645	0.3612787592	-1.3466961235
C	-1.2947480871	-0.9958271962	-1.6169899466
C	-1.0733520885	-1.75079439	-0.4223546745
B	0.0326458919	1.8382814532	0.7714855603
N	1.312393974	2.4035755513	0.0298835621
C	1.6415358532	3.6783645465	-0.2504254377
C	2.9013928042	3.6974353664	-0.8517608516
C	3.2725781699	2.3467631223	-0.901313396
N	2.3125403472	1.5711640234	-0.3668855391
Li	1.7861867774	-0.2853364076	-0.0460166096
O	2.6891244303	-1.78668339	-1.0328526883
C	3.1733477131	-2.7449992687	-0.092381107
C	3.7137560943	-1.9777446995	1.0992538658
O	2.6740322797	-1.1234601136	1.5626142328
C	3.0433540592	-0.3093511472	2.6809485793
C	2.2465337363	-2.3573380372	-2.265143768
H	-1.0178685186	1.1834377314	-2.0475753514
H	-1.7045199225	-1.3771079819	-2.5452957265
H	-1.2863524771	-2.8042629239	-0.2817648085
H	-0.3464308944	-1.0994048304	1.5996267805
H	-0.7894347605	2.7328730988	0.7477741211
H	0.3459307333	1.573286478	1.9272465101
H	0.9612862996	4.4824199521	-0.0058801001
H	4.173273103	1.8972455156	-1.302356688
H	2.3532585103	-3.4122046497	0.2108017704

C	-3.689327919	-0.2775278958	1.5754581837
H	3.974797036	-3.3487611955	-0.5428537078
H	1.887460993	-1.533236728	-2.883396394
H	3.0806666648	-2.8638564791	-2.7689533316
H	1.4275687344	-3.0672260429	-2.0931272154
H	4.5869967155	-1.3759040708	0.8052218958
H	4.018951647	-2.679375965	1.8901045137
H	3.9062059635	0.320788119	2.4298773822
H	2.1837702659	0.3251323844	2.9021382075
H	3.281204259	-0.9432661718	3.5456297668
H	-3.3988083341	-0.618460811	2.5613663508
H	-3.1213301253	1.8928642956	1.606183743
H	-4.0035366522	1.9218196558	-0.9390570938
H	-4.794460801	-0.5832951537	-1.5808538028
H	-4.4204166327	-2.154457606	0.5856740163
H	3.4531696335	4.5570818018	-1.2058667399

The full refernces (46) and (47) read as follows:

(46) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Montgomery, J. A.; Stratmann, R. E.; Burant, J. C.; Dapprich, S.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; Mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B. G.; Chen, W.; Wong, M. W.; Andres, J. L.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. *Gaussian 98, Revision A.11*, Gaussian, Inc.: Pittsburgh, PA, 1998.

(47) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; J. A. Montgomery, J.; 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.; Bakken, V.; 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.