

Supplementary Material for manuscript:

## **Group-10 $\pi$ -hole $\cdots$ d<sub>z<sup>2</sup></sub> [M<sup>II</sup>] interactions: a theoretical study of model systems inspired by CSD structures.**

**Miriam Calabrese<sup>a</sup>, Sergi Burguera<sup>b</sup>, Giuseppe Resnati<sup>a,\*</sup> and Antonio Frontera<sup>b,\*</sup>**

<sup>a</sup>*NFMLab, Department of Chemistry, Materials, and Chemical Engineering "Giulio Natta", Politecnico di Milano, via L. Mancinelli 7, I-20131 Milano, Italy,  
E-mail: giuseppe.resnati@polimi.it.*

<sup>b</sup>*Departament de Química, Universitat de les Illes Balears, Crta de Valldemossa Km, 7.5, 07122 Palma de mallorca (Balears), SPAIN.  
E-mail: [toni.frontera@uib.es](mailto:toni.frontera@uib.es)*

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### Cartesian coordinates of complexes 11-34

#### 11a.

C	-2.5060253	1.2081836	-1.3833788
H	-3.0921896	2.1349602	-1.3780993
C	-3.1918590	-0.0000925	-1.3504988
H	-4.2722430	-0.0001648	-1.3221749
C	-2.5059769	-1.2083352	-1.3832349
H	-3.0920541	-2.1351695	-1.3777997
O	-1.2591033	1.3695477	-1.4224110
O	-1.2590568	-1.3695799	-1.4222983
C	2.5060253	-1.2081836	-1.3833788
H	3.0921896	-2.1349602	-1.3780993
C	3.1918590	0.0000925	-1.3504988
H	4.2722430	0.0001648	-1.3221749
C	2.5059769	1.2083352	-1.3832349
H	3.0920541	2.1351695	-1.3777997
O	1.2591033	-1.3695477	-1.4224110
O	1.2590568	1.3695799	-1.4222983
Ni	0.0000000	0.0000000	-1.4122402
C	-1.3875158	0.0000985	1.9677005
C	-0.6937867	-1.2016959	1.9638360
C	0.6936265	-1.2017846	1.9638373
C	1.3875158	-0.0000985	1.9677005
C	0.6937867	1.2016959	1.9638360
C	-0.6936265	1.2017846	1.9638373
H	-1.2346741	-2.1407982	1.9471541
H	1.2343838	-2.1409731	1.9471678
H	1.2346741	2.1407982	1.9471541
H	-1.2343838	2.1409731	1.9471678
H	-2.4713514	0.0001625	1.9563200
H	2.4713514	-0.0001625	1.9563200

#### 11b.

C	2.5054179	-1.2083680	1.3716794
H	3.0914903	-2.1351480	1.3632979
C	3.1909741	-0.0000779	1.3329421
H	4.2710618	-0.0001852	1.2963364
C	2.5055125	1.2082200	1.3716146
H	3.0916391	2.1349813	1.3630665
O	1.2588918	-1.3698110	1.4199204
O	1.2589721	1.3697673	1.4199224
C	-2.5054179	1.2083680	1.3716794
H	-3.0914903	2.1351480	1.3632979
C	-3.1909741	0.0000779	1.3329421
H	-4.2710618	0.0001852	1.2963364
C	-2.5055125	-1.2082200	1.3716146
H	-3.0916391	-2.1349813	1.3630665
O	-1.2588918	1.3698110	1.4199204
O	-1.2589721	-1.3697673	1.4199224
C	0.0000835	-1.3882621	-1.9468468
C	1.2011189	-0.6936947	-1.9503497
C	1.2010844	0.6937966	-1.9503496
C	-0.0000835	1.3882621	-1.9468468
C	-1.2011189	0.6936947	-1.9503497
C	-1.2010844	-0.6937966	-1.9503496
Ni	0.0000000	0.0000000	1.4111627
H	-2.1403496	-1.2348664	-1.9362739
H	-2.1404564	1.2347090	-1.9362749
H	2.1403496	1.2348664	-1.9362739
H	2.1404564	-1.2347090	-1.9362749
H	0.0000855	-2.4715681	-1.9242661
H	-0.0000855	2.4715681	-1.9242661

**12a.**

C	-2.5067862	1.2074402	-1.4214518
H	-3.0920996	2.1343124	-1.4262992
C	-3.1921862	0.0000000	-1.4430099
H	-4.2724880	0.0000000	-1.4582926

C	-2.5067862	-1.2074402	-1.4214518
H	-3.0920996	-2.1343124	-1.4262992
O	-1.2580506	1.3692861	-1.3932533
O	-1.2580506	-1.3692861	-1.3932533
C	2.5067862	-1.2074402	-1.4214518
H	3.0920996	-2.1343124	-1.4262992
C	3.1921862	0.0000000	-1.4430099
H	4.2724880	0.0000000	-1.4582926
C	2.5067862	1.2074402	-1.4214518
H	3.0920996	2.1343124	-1.4262992
O	1.2580506	-1.3692861	-1.3932533
O	1.2580506	1.3692861	-1.3932533
Ni	0.0000000	0.0000000	-1.3856312
C	-1.3615429	0.0000000	2.0239232
C	-0.6930909	-1.2084438	2.0169615
C	0.6930909	-1.2084438	2.0169615
C	1.3615429	-0.0000000	2.0239232
C	0.6930909	1.2084438	2.0169615
C	-0.6930909	1.2084438	2.0169615
H	-1.2547224	-2.1332913	1.9972335
H	1.2547224	-2.1332913	1.9972335
H	1.2547224	2.1332913	1.9972335
H	-1.2547224	2.1332913	1.9972335
F	-2.7024881	0.0000000	2.0238133
F	2.7024881	0.0000000	2.0238133

**12b.**

C	2.5053266	-1.2084848	1.3700506
H	3.0897284	-2.1360673	1.3611139
C	3.1910485	0.0000000	1.3326747
H	4.2712349	0.0000000	1.2997240
C	2.5053266	1.2084848	1.3700506
H	3.0897284	2.1360673	1.3611139
O	1.2581685	-1.3686434	1.4159067
O	1.2581685	1.3686434	1.4159067

C	-2.5053266	1.2084848	1.3700506
H	-3.0897284	2.1360673	1.3611139
C	-3.1910485	0.0000000	1.3326747
H	-4.2712349	0.0000000	1.2997240
C	-2.5053266	-1.2084848	1.3700506
H	-3.0897284	-2.1360673	1.3611139
O	-1.2581685	1.3686434	1.4159067
O	-1.2581685	-1.3686434	1.4159067
C	0.0000000	-1.3637443	-1.9438453
C	1.2076308	-0.6931899	-1.9444101
C	1.2076308	0.6931899	-1.9444101
C	0.0000000	1.3637443	-1.9438453
C	-1.2076308	0.6931899	-1.9444101
C	-1.2076308	-0.6931899	-1.9444101
Ni	0.0000000	0.0000000	1.4139006
F	0.0000000	2.7018203	-1.9372323
F	0.0000000	-2.7018203	-1.9372323
H	-2.1327137	-1.2549489	-1.9317968
H	-2.1327137	1.2549489	-1.9317968
H	2.1327137	1.2549489	-1.9317968
H	2.1327137	-1.2549489	-1.9317968

**13a.**

C	-2.5053037	1.2087673	-1.3309332
H	-3.0881660	2.1365838	-1.3108839
C	-3.1896623	-0.0003748	-1.2829058
H	-4.2691919	-0.0005344	-1.2323193
C	-2.5050339	-1.2093398	-1.3309674
H	-3.0877529	-2.1372437	-1.3109163
O	-1.2582664	1.3678770	-1.3955869
O	-1.2579440	-1.3682139	-1.3956230
C	2.5053037	-1.2087673	-1.3309332
H	3.0881660	-2.1365838	-1.3108839
C	3.1896623	0.0003748	-1.2829058
H	4.2691919	0.0005344	-1.2323193

C	2.5050339	1.2093398	-1.3309674
H	3.0877529	2.1372437	-1.3109163
O	1.2582664	-1.3678770	-1.3955869
O	1.2579440	1.3682139	-1.3956230
Ni	0.0000000	0.0000000	-1.4050789
C	-1.3904641	0.0004233	1.8915005
C	-0.6930857	-1.1911799	1.8874105
C	0.6923861	-1.1916160	1.8874406
C	1.3904641	-0.0004233	1.8915005
C	0.6930857	1.1911799	1.8874105
C	-0.6923861	1.1916160	1.8874406
F	-1.3539690	-2.3448298	1.8757951
F	1.3525470	-2.3456764	1.8759087
F	1.3539690	2.3448298	1.8757951
F	-1.3525470	2.3456764	1.8759087
H	-2.4719333	0.0007157	1.8746198
H	2.4719333	-0.0007157	1.8746198

**13b.**

C	2.5073606	-1.2080515	1.3562691
H	3.0915551	-2.1348899	1.3397069
C	3.1921608	-0.0001046	1.3441763
H	4.2721029	-0.0001290	1.3142173
C	2.5074245	1.2078552	1.3562178
H	3.0916742	2.1346626	1.3397231
O	1.2578269	-1.3694221	1.3803399
O	1.2578942	1.3693261	1.3801734
C	-2.5073606	1.2080515	1.3562691
H	-3.0915551	2.1348899	1.3397069
C	-3.1921608	0.0001046	1.3441763
H	-4.2721029	0.0001290	1.3142173
C	-2.5074245	-1.2078552	1.3562178
H	-3.0916742	-2.1346626	1.3397231
O	-1.2578269	1.3694221	1.3803399
O	-1.2578942	-1.3693261	1.3801734

C	0.0001778	-1.3920189	-1.9220074
C	1.1900044	-0.6926237	-1.9267894
C	1.1898242	0.6929184	-1.9267748
C	-0.0001778	1.3920189	-1.9220074
C	-1.1900044	0.6926237	-1.9267894
C	-1.1898242	-0.6929184	-1.9267748
Ni	0.0000000	0.0000000	1.3895936
H	-0.0003082	2.4731971	-1.8952086
H	0.0003082	-2.4731971	-1.8952086
F	-2.3465372	1.3509742	-1.9174307
F	-2.3462010	-1.3515239	-1.9174097
F	2.3462010	1.3515239	-1.9174097
F	2.3465372	-1.3509742	-1.9174307

**14a.**

C	-2.5073950	1.2077864	-1.3858069
H	-3.0904585	2.1354178	-1.3862820
C	-3.1918683	-0.0000942	-1.4195386
H	-4.2718947	-0.0001957	-1.4467755
C	-2.5072378	-1.2078638	-1.3858177
H	-3.0901297	-2.1355905	-1.3863226
O	-1.2576997	1.3676539	-1.3453627
O	-1.2575277	-1.3676513	-1.3453098
C	2.5073950	-1.2077864	-1.3858069
H	3.0904585	-2.1354178	-1.3862820
C	3.1918683	0.0000942	-1.4195386
H	4.2718947	0.0001957	-1.4467755
C	2.5072378	1.2078638	-1.3858177
H	3.0901297	2.1355905	-1.3863226
O	1.2576997	-1.3676539	-1.3453627
O	1.2575277	1.3676513	-1.3453098
Ni	0.0000000	0.0000000	-1.3514030
C	-1.3833646	0.0000922	1.9707690
C	-0.6928289	-1.2011661	1.9629083
C	0.6926560	-1.2012534	1.9628910

C	1.3833646	-0.0000922	1.9707690
C	0.6928289	1.2011661	1.9629083
C	-0.6926560	1.2012534	1.9628910
F	-2.7069184	0.0001955	1.9755736
F	2.7069184	-0.0001955	1.9755736
F	-1.3585195	-2.3431893	1.9524224
F	-1.3582041	2.3433683	1.9523529
F	1.3585195	2.3431893	1.9524224
F	1.3582041	-2.3433683	1.9523529

**14b.**

C	2.5075443	-1.2080992	1.3495659
H	3.0902201	-2.1357523	1.3345217
C	3.1926938	-0.0001497	1.3426676
H	4.2728965	-0.0001411	1.3218594
C	2.5075868	1.2080391	1.3495478
H	3.0903350	2.1355854	1.3345046
O	1.2573303	-1.3683027	1.3654043
O	1.2574579	1.3681869	1.3652820
C	-2.5075443	1.2080992	1.3495659
H	-3.0902201	2.1357523	1.3345217
C	-3.1926938	0.0001497	1.3426676
H	-4.2728965	0.0001411	1.3218594
C	-2.5075868	-1.2080391	1.3495478
H	-3.0903350	-2.1355854	1.3345046
O	-1.2573303	1.3683027	1.3654043
O	-1.2574579	-1.3681869	1.3652820
C	0.0001473	-1.3868377	-1.9106153
C	1.1992808	-0.6927695	-1.9146908
C	1.1991350	0.6929608	-1.9146472
C	-0.0001473	1.3868377	-1.9106153
C	-1.1992808	0.6927695	-1.9146908
C	-1.1991350	-0.6929608	-1.9146472
Ni	0.0000000	0.0000000	1.3789013
F	-0.0002687	2.7074680	-1.8984688



F	0.0002687	-2.7074680	-1.8984688
F	-2.3444123	1.3561149	-1.9072208
F	-2.3441682	-1.3564832	-1.9071611
F	2.3444123	-1.3561149	-1.9072208
F	2.3441682	1.3564832	-1.9071611

**15a.**

C	-2.5833075	1.2299523	-1.4033939
H	-3.2126164	2.1280101	-1.3968816
C	-3.2350264	0.0000000	-1.3842276
H	-4.3164189	0.0000000	-1.3672135
C	-2.5833075	-1.2299523	-1.4033939
H	-3.2126164	-2.1280101	-1.3968816
O	-1.3477755	1.4608763	-1.4291782
O	-1.3477755	-1.4608763	-1.4291782
C	2.5833075	-1.2299523	-1.4033939
H	3.2126164	-2.1280101	-1.3968816
C	3.2350264	-0.0000000	-1.3842276
H	4.3164189	0.0000000	-1.3672135
C	2.5833075	1.2299523	-1.4033939
H	3.2126164	2.1280101	-1.3968816
O	1.3477755	-1.4608763	-1.4291782
O	1.3477755	1.4608763	-1.4291782
C	-1.3874078	0.0000000	1.9963620
C	-0.6936991	-1.2017959	1.9934020
C	0.6936991	-1.2017959	1.9934020
C	1.3874078	-0.0000000	1.9963620
C	0.6936991	1.2017959	1.9934020
C	-0.6936991	1.2017959	1.9934020
Pd	0.0000000	0.0000000	-1.4283543
H	-1.2345127	-2.1408845	1.9777144
H	-1.2345127	2.1408845	1.9777144
H	1.2345127	-2.1408845	1.9777144
H	1.2345127	2.1408845	1.9777144
H	-2.4713149	0.0000000	1.9859310

H	2.4713149	0.0000000	1.9859310
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**15b.**

C	2.5825792	-1.2298227	1.3951022
H	3.2116282	-2.1279538	1.3791722
C	3.2336626	0.0000000	1.3574583
H	4.3143453	0.0000000	1.3158483
C	2.5825792	1.2298227	1.3951022
H	3.2116282	2.1279538	1.3791722
O	1.3479046	-1.4606447	1.4482116
O	1.3479046	1.4606447	1.4482116
C	-2.5825792	1.2298227	1.3951022
H	-3.2116282	2.1279538	1.3791722
C	-3.2336626	0.0000000	1.3574583
H	-4.3143453	-0.0000000	1.3158483
C	-2.5825792	-1.2298227	1.3951022
H	-3.2116282	-2.1279538	1.3791722
O	-1.3479046	1.4606447	1.4482116
O	-1.3479046	-1.4606447	1.4482116
C	0.0000000	-1.3882892	-1.9788061
C	1.2012225	-0.6938161	-1.9817776
C	1.2012225	0.6938161	-1.9817776
C	0.0000000	1.3882892	-1.9788061
C	-1.2012225	0.6938161	-1.9817776
C	-1.2012225	-0.6938161	-1.9817776
H	-2.1404995	1.2351057	-1.9706533
H	-2.1404995	-1.2351057	-1.9706533
H	2.1404995	1.2351057	-1.9706533
H	2.1404995	-1.2351057	-1.9706533
H	0.0000000	2.4717668	-1.9602864
H	-0.0000000	-2.4717668	-1.9602864
Pd	0.0000000	0.0000000	1.4513512

**16a.**

C	-2.5847732	1.2288748	-1.4450614
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H	-3.2128073	2.1274043	-1.4441153
C	-3.2361205	-0.0000000	-1.4514525
H	-4.3172893	-0.0000000	-1.4486153
C	-2.5847732	-1.2288748	-1.4450614
H	-3.2128073	-2.1274043	-1.4441153
O	-1.3475489	1.4602035	-1.4389246
O	-1.3475489	-1.4602035	-1.4389246
C	2.5847732	-1.2288748	-1.4450614
H	3.2128073	-2.1274043	-1.4441153
C	3.2361205	0.0000000	-1.4514525
H	4.3172893	-0.0000000	-1.4486153
C	2.5847732	1.2288748	-1.4450614
H	3.2128073	2.1274043	-1.4441153
O	1.3475489	-1.4602035	-1.4389246
O	1.3475489	1.4602035	-1.4389246
C	-1.3612691	0.0000000	2.0542061
C	-0.6931486	-1.2086511	2.0506041
C	0.6931486	-1.2086511	2.0506041
C	1.3612691	0.0000000	2.0542061
C	0.6931486	1.2086511	2.0506041
C	-0.6931486	1.2086511	2.0506041
Pd	0.0000000	0.0000000	-1.4381068
F	-2.7024217	0.0000000	2.0502957
F	2.7024217	0.0000000	2.0502957
H	-1.2556139	-2.1332826	2.0348070
H	-1.2556139	2.1332826	2.0348070
H	1.2556139	-2.1332826	2.0348070
H	1.2556139	2.1332826	2.0348070

**16b.**

C	2.5825962	-1.2299584	1.3885083
H	3.2100506	-2.1289891	1.3717591
C	3.2339454	0.0000000	1.3510578
H	4.3147520	0.0000000	1.3124408
C	2.5825962	1.2299584	1.3885083

H	3.2100506	2.1289891	1.3717591
O	1.3473734	-1.4595238	1.4407131
O	1.3473734	1.4595238	1.4407131
C	-2.5825962	1.2299584	1.3885083
H	-3.2100506	2.1289891	1.3717591
C	-3.2339454	0.0000000	1.3510578
H	-4.3147520	0.0000000	1.3124408
C	-2.5825962	-1.2299584	1.3885083
H	-3.2100506	-2.1289891	1.3717591
O	-1.3473734	1.4595238	1.4407131
O	-1.3473734	-1.4595238	1.4407131
C	0.0000000	-1.3635535	-1.9694364
C	1.2078257	-0.6932338	-1.9697312
C	1.2078257	0.6932338	-1.9697312
C	0.0000000	1.3635535	-1.9694364
C	-1.2078257	0.6932338	-1.9697312
C	-1.2078257	-0.6932338	-1.9697312
H	-2.1327607	1.2554041	-1.9585430
H	-2.1327607	-1.2554041	-1.9585430
H	2.1327607	1.2554041	-1.9585430
H	2.1327607	-1.2554041	-1.9585430
Pd	0.0000000	0.0000000	1.4484209
F	0.0000000	2.7017513	-1.9636853
F	0.0000000	-2.7017513	-1.9636853

**17a.**

C	-2.5817681	1.2304118	-1.3548254
H	-3.2075485	2.1298419	-1.3279762
C	-3.2318909	0.0000000	-1.3066106
H	-4.3119813	-0.0000000	-1.2513251
C	-2.5817681	-1.2304118	-1.3548254
H	-3.2075485	-2.1298419	-1.3279762
O	-1.3468157	1.4589756	-1.4254449
O	-1.3468157	-1.4589756	-1.4254449
C	2.5817681	-1.2304118	-1.3548254

H	3.2075485	-2.1298419	-1.3279762
C	3.2318909	0.0000000	-1.3066106
H	4.3119813	-0.0000000	-1.2513251
C	2.5817681	1.2304118	-1.3548254
H	3.2075485	2.1298419	-1.3279762
O	1.3468157	-1.4589756	-1.4254449
O	1.3468157	1.4589756	-1.4254449
C	-1.3906341	0.0000000	1.9239450
C	-0.6927704	-1.1913478	1.9205378
C	0.6927704	-1.1913478	1.9205378
C	1.3906341	0.0000000	1.9239450
C	0.6927704	1.1913478	1.9205378
C	-0.6927704	1.1913478	1.9205378
F	-1.3531348	2.3453910	1.9107011
F	-1.3531348	-2.3453910	1.9107011
F	1.3531348	-2.3453910	1.9107011
F	1.3531348	2.3453910	1.9107011
H	-2.4723105	0.0000000	1.9096362
H	2.4723105	-0.0000000	1.9096362
Pd	0.0000000	0.0000000	-1.4432605

**17b.**

C	2.5838911	-1.2294493	1.3680503
H	3.2109828	-2.1276981	1.3404553
C	3.2339497	0.0000000	1.3428648
H	4.3139386	-0.0000000	1.2921952
C	2.5838911	1.2294493	1.3680503
H	3.2109828	2.1276981	1.3404553
O	1.3469727	-1.4604210	1.4156013
O	1.3469727	1.4604210	1.4156013
C	-2.5838911	1.2294493	1.3680503
H	-3.2109828	2.1276981	1.3404553
C	-3.2339497	0.0000000	1.3428648
H	-4.3139386	0.0000000	1.2921952
C	-2.5838911	-1.2294493	1.3680503

H	-3.2109828	-2.1276981	1.3404553
O	-1.3469727	1.4604210	1.4156013
O	-1.3469727	-1.4604210	1.4156013
C	-0.0000000	-1.3923663	-1.9394066
C	1.1897255	-0.6927869	-1.9425101
C	1.1897255	0.6927869	-1.9425101
C	-0.0000000	1.3923663	-1.9394066
C	-1.1897255	0.6927869	-1.9425101
C	-1.1897255	-0.6927869	-1.9425101
Pd	-0.0000000	0.0000000	1.4349897
F	2.3466441	1.3506686	-1.9313089
F	2.3466441	-1.3506686	-1.9313089
F	-2.3466441	-1.3506686	-1.9313089
F	-2.3466441	1.3506686	-1.9313089
H	0.0000000	2.4736486	-1.9137242
H	-0.0000000	-2.4736486	-1.9137242

**18a.**

C	-2.5849146	1.2292840	-1.4036366
H	-3.2107891	2.1287415	-1.4003611
C	-3.2357314	0.0000000	-1.4253081
H	-4.3168331	0.0000000	-1.4400434
C	-2.5849146	-1.2292840	-1.4036366
H	-3.2107891	-2.1287415	-1.4003611
O	-1.3467451	1.4587315	-1.3804659
O	-1.3467451	-1.4587315	-1.3804659
C	2.5849146	-1.2292840	-1.4036366
H	3.2107891	-2.1287415	-1.4003611
C	3.2357314	-0.0000000	-1.4253081
H	4.3168331	0.0000000	-1.4400434
C	2.5849146	1.2292840	-1.4036366
H	3.2107891	2.1287415	-1.4003611
O	1.3467451	-1.4587315	-1.3804659
O	1.3467451	1.4587315	-1.3804659
C	-1.3833331	0.0000000	1.9950552
C	-0.6927361	-1.2012146	1.9903325

C	0.6927361	-1.2012146	1.9903325
C	1.3833331	0.0000000	1.9950552
C	0.6927361	1.2012146	1.9903325
C	-0.6927361	1.2012146	1.9903325
F	-1.3583415	2.3434268	1.9801970
F	-1.3583415	-2.3434268	1.9801970
F	1.3583415	-2.3434268	1.9801970
F	1.3583415	2.3434268	1.9801970
Pd	0.0000000	0.0000000	-1.3903626
F	-2.7070410	-0.0000000	1.9933458
F	2.7070410	0.0000000	1.9933458

**18b.**

C	2.5841054	-1.2295371	1.3616950
H	3.2097664	-2.1286895	1.3365919
C	3.2344856	0.0000000	1.3387038
H	4.3147531	-0.0000000	1.2941661
C	2.5841054	1.2295371	1.3616950
H	3.2097664	2.1286895	1.3365919
O	1.3465311	-1.4592928	1.4034786
O	1.3465311	1.4592928	1.4034786
C	-2.5841054	1.2295371	1.3616950
H	-3.2097664	2.1286895	1.3365919
C	-3.2344856	-0.0000000	1.3387038
H	-4.3147531	0.0000000	1.2941661
C	-2.5841054	-1.2295371	1.3616950
H	-3.2097664	-2.1286895	1.3365919
O	-1.3465311	1.4592928	1.4034786
O	-1.3465311	-1.4592928	1.4034786
C	0.0000000	-1.3866956	-1.9279686
C	1.1992511	-0.6928440	-1.9304787
C	1.1992511	0.6928440	-1.9304787
C	0.0000000	1.3866956	-1.9279686
C	-1.1992511	0.6928440	-1.9304787
C	-1.1992511	-0.6928440	-1.9304787

Pd	0.0000000	0.0000000	1.4243515
F	-0.0000000	2.7074705	-1.9166718
F	-0.0000000	-2.7074705	-1.9166718
F	2.3445517	1.3560677	-1.9214895
F	2.3445517	-1.3560677	-1.9214895
F	-2.3445517	-1.3560677	-1.9214895
F	-2.3445517	1.3560677	-1.9214895

**19a.**

C	-2.5796370	1.2327730	-1.3933425
H	-3.2052045	2.1309436	-1.3825278
C	-3.2239030	0.0000000	-1.3704015
H	-4.3052678	-0.0000000	-1.3454548
C	-2.5796370	-1.2327730	-1.3933425
H	-3.2052045	-2.1309436	-1.3825278
O	-1.3404680	1.4679992	-1.4265277
O	-1.3404680	-1.4679992	-1.4265277
C	2.5796370	-1.2327730	-1.3933425
H	3.2052045	-2.1309436	-1.3825278
C	3.2239030	0.0000000	-1.3704015
H	4.3052678	0.0000000	-1.3454548
C	2.5796370	1.2327730	-1.3933425
H	3.2052045	2.1309436	-1.3825278
O	1.3404680	-1.4679992	-1.4265277
O	1.3404680	1.4679992	-1.4265277
C	-1.3871844	-0.0000000	1.9815769
C	-0.6936124	-1.2016497	1.9790137
C	0.6936124	-1.2016497	1.9790137
C	1.3871844	0.0000000	1.9815769
C	0.6936124	1.2016497	1.9790137
C	-0.6936124	1.2016497	1.9790137
H	-1.2345918	-2.1408107	1.9630440
H	-1.2345918	2.1408107	1.9630440
H	1.2345918	-2.1408107	1.9630440
H	1.2345918	2.1408107	1.9630440



H	-2.4711989	-0.0000000	1.9703439
H	2.4711989	0.0000000	1.9703439
Pt	0.0000000	0.0000000	-1.4307680

**19b.**

C	2.5793898	-1.2327808	1.3902348
H	3.2050143	-2.1309277	1.3782532
C	3.2235955	0.0000000	1.3649729
H	4.3048785	0.0000000	1.3371995
C	2.5793898	1.2327808	1.3902348
H	3.2050143	2.1309277	1.3782532
O	1.3403382	-1.4681006	1.4269516
O	1.3403382	1.4681006	1.4269516
C	-2.5793898	1.2327808	1.3902348
H	-3.2050143	2.1309277	1.3782532
C	-3.2235955	0.0000000	1.3649729
H	-4.3048785	0.0000000	1.3371995
C	-2.5793898	-1.2327808	1.3902348
H	-3.2050143	-2.1309277	1.3782532
O	-1.3403382	1.4681006	1.4269516
O	-1.3403382	-1.4681006	1.4269516
C	0.0000000	-1.3880175	-1.9736186
C	1.2009866	-0.6936909	-1.9762739
C	1.2009866	0.6936909	-1.9762739
C	0.0000000	1.3880175	-1.9736186
C	-1.2009866	0.6936909	-1.9762739
C	-1.2009866	-0.6936909	-1.9762739
Pt	0.0000000	0.0000000	1.4318529
H	-2.1402536	1.2350969	-1.9646560
H	-2.1402536	-1.2350969	-1.9646560
H	2.1402536	1.2350969	-1.9646560
H	2.1402536	-1.2350969	-1.9646560
H	-0.0000000	2.4715079	-1.9534996
H	-0.0000000	-2.4715079	-1.9534996

**20a.**

C	-2.5814639	1.2317572	-1.4264520
H	-3.2064415	2.1299231	-1.4267584
C	-3.2253635	0.0000000	-1.4391173
H	-4.3066913	-0.0000000	-1.4444112
C	-2.5814639	-1.2317572	-1.4264520
H	-3.2064415	-2.1299231	-1.4267584
O	-1.3405984	1.4675417	-1.4121768
O	-1.3405984	-1.4675417	-1.4121768
C	2.5814639	-1.2317572	-1.4264520
H	3.2064415	-2.1299231	-1.4267584
C	3.2253635	0.0000000	-1.4391173
H	4.3066913	0.0000000	-1.4444112
C	2.5814639	1.2317572	-1.4264520
H	3.2064415	2.1299231	-1.4267584
O	1.3405984	-1.4675417	-1.4121768
O	1.3405984	1.4675417	-1.4121768
C	-1.3603616	0.0000000	2.0300542
C	-0.6929198	-1.2086155	2.0239558
C	0.6929198	-1.2086155	2.0239558
C	1.3603616	0.0000000	2.0300542
C	0.6929198	1.2086155	2.0239558
C	-0.6929198	1.2086155	2.0239558
H	-1.2551919	-2.1332327	2.0055214
H	-1.2551919	2.1332327	2.0055214
H	1.2551919	-2.1332327	2.0055214
H	1.2551919	2.1332327	2.0055214
Pt	0.0000000	0.0000000	-1.4117845
F	-2.7018622	0.0000000	2.0311865
F	2.7018622	0.0000000	2.0311865

**20b.**

C	2.5793272	-1.2329309	1.3825232
H	3.2034592	-2.1318512	1.3661317
C	3.2234357	0.0000000	1.3508896

H	4.3045429	0.0000000	1.3166131
C	2.5793272	1.2329309	1.3825232
H	3.2034592	2.1318512	1.3661317
O	1.3401500	-1.4672233	1.4283341
O	1.3401500	1.4672233	1.4283341
C	-2.5793272	1.2329309	1.3825232
H	-3.2034592	2.1318512	1.3661317
C	-3.2234357	0.0000000	1.3508896
H	-4.3045429	0.0000000	1.3166131
C	-2.5793272	-1.2329309	1.3825232
H	-3.2034592	-2.1318512	1.3661317
O	-1.3401500	1.4672233	1.4283341
O	-1.3401500	-1.4672233	1.4283341
C	0.0000000	-1.3631912	-1.9610971
C	1.2075636	-0.6930940	-1.9625069
C	1.2075636	0.6930940	-1.9625069
C	0.0000000	1.3631912	-1.9610971
C	-1.2075636	0.6930940	-1.9625069
C	-1.2075636	-0.6930940	-1.9625069
Pt	0.0000000	0.0000000	1.4364835
F	-0.0000000	-2.7017775	-1.9517689
F	0.0000000	2.7017775	-1.9517689
H	-2.1324430	1.2553690	-1.9509213
H	-2.1324430	-1.2553690	-1.9509213
H	2.1324430	1.2553690	-1.9509213
H	2.1324430	-1.2553690	-1.9509213

**21a.**

C	-2.5788801	1.2334034	-1.3551418
H	-3.2016470	2.1326100	-1.3305856
C	-3.2216994	0.0000000	-1.3118449
H	-4.3021117	0.0000000	-1.2605972
C	-2.5788801	-1.2334034	-1.3551418
H	-3.2016470	-2.1326100	-1.3305856
O	-1.3399259	1.4669686	-1.4190450

O	-1.3399259	-1.4669686	-1.4190450
C	2.5788801	-1.2334034	-1.3551418
H	3.2016470	-2.1326100	-1.3305856
C	3.2216994	0.0000000	-1.3118449
H	4.3021117	0.0000000	-1.2605972
C	2.5788801	1.2334034	-1.3551418
H	3.2016470	2.1326100	-1.3305856
O	1.3399259	-1.4669686	-1.4190450
O	1.3399259	1.4669686	-1.4190450
C	-1.3902759	0.0000000	1.9253605
C	-0.6925469	-1.1910131	1.9215806
C	0.6925469	-1.1910131	1.9215806
C	1.3902759	0.0000000	1.9253605
C	0.6925469	1.1910131	1.9215806
C	-0.6925469	1.1910131	1.9215806
Pt	0.0000000	0.0000000	-1.4337330
F	-1.3530905	-2.3455117	1.9099155
F	1.3530905	-2.3455117	1.9099155
F	1.3530905	2.3455117	1.9099155
F	-1.3530905	2.3455117	1.9099155
H	-2.4719092	0.0000000	1.9105007
H	2.4719092	0.0000000	1.9105007

**21b.**

C	2.5810917	1.2324917	1.3712609
H	3.2054202	2.1304942	1.3504770
C	3.2239699	0.0000000	1.3572328
H	4.3047382	0.0000000	1.3212100
C	2.5810917	-1.2324917	1.3712609
H	3.2054202	-2.1304942	1.3504770
O	1.3400477	1.4683786	1.4011419
O	1.3400477	-1.4683786	1.4011419
C	-2.5810917	-1.2324917	1.3712609
H	-3.2054202	-2.1304942	1.3504770
C	-3.2239699	0.0000000	1.3572328

H	-4.3047382	0.0000000	1.3212100
C	-2.5810917	1.2324917	1.3712609
H	-3.2054202	2.1304942	1.3504770
O	-1.3400477	-1.4683786	1.4011419
O	-1.3400477	1.4683786	1.4011419
C	-0.0000000	1.3922542	-1.9470960
C	1.1892940	0.6925882	-1.9485296
C	1.1892940	-0.6925882	-1.9485296
C	-0.0000000	-1.3922542	-1.9470960
C	-1.1892940	-0.6925882	-1.9485296
C	-1.1892940	0.6925882	-1.9485296
Pt	-0.0000000	0.0000000	1.4142882
F	2.3468182	1.3503948	-1.9338325
F	2.3468182	-1.3503948	-1.9338325
F	-2.3468182	-1.3503948	-1.9338325
F	-2.3468182	1.3503948	-1.9338325
H	0.0000000	2.4735236	-1.9195264
H	0.0000000	-2.4735236	-1.9195264

**22a.**

C	-2.5818309	1.2324215	-1.3929371
H	-3.2047681	2.1315279	-1.3836550
C	-3.2251992	-0.0000000	-1.3951260
H	-4.3065123	0.0000000	-1.3849223
C	-2.5818309	-1.2324215	-1.3929371
H	-3.2047681	-2.1315279	-1.3836550
O	-1.3399375	1.4671281	-1.3953035
O	-1.3399375	-1.4671281	-1.3953035
C	2.5818309	-1.2324215	-1.3929371
H	3.2047681	-2.1315279	-1.3836550
C	3.2251992	-0.0000000	-1.3951260
H	4.3065123	0.0000000	-1.3849223
C	2.5818309	1.2324215	-1.3929371
H	3.2047681	2.1315279	-1.3836550
O	1.3399375	-1.4671281	-1.3953035

O	1.3399375	1.4671281	-1.3953035
C	-1.3827952	0.0000000	1.9806128
C	-0.6924907	-1.2008062	1.9735928
C	0.6924907	-1.2008062	1.9735928
C	1.3827952	0.0000000	1.9806128
C	0.6924907	1.2008062	1.9735928
C	-0.6924907	1.2008062	1.9735928
Pt	0.0000000	0.0000000	-1.4023691
F	-2.7068833	0.0000000	1.9805684
F	2.7068833	-0.0000000	1.9805684
F	-1.3584336	-2.3433507	1.9583285
F	1.3584336	-2.3433507	1.9583285
F	1.3584336	2.3433507	1.9583285
F	-1.3584336	2.3433507	1.9583285

**22b.**

C	2.5808294	-1.2326261	1.3609355
H	3.2037318	-2.1313820	1.3371576
C	3.2233983	0.0000000	1.3337245
H	4.3036650	-0.0000000	1.2852223
C	2.5808294	1.2326261	1.3609355
H	3.2037318	2.1313820	1.3371576
O	1.3399107	-1.4676115	1.4066127
O	1.3399107	1.4676115	1.4066127
C	-2.5808294	1.2326261	1.3609355
H	-3.2037318	2.1313820	1.3371576
C	-3.2233983	0.0000000	1.3337245
H	-4.3036650	0.0000000	1.2852223
C	-2.5808294	-1.2326261	1.3609355
H	-3.2037318	-2.1313820	1.3371576
O	-1.3399107	1.4676115	1.4066127
O	-1.3399107	-1.4676115	1.4066127
C	0.0000000	-1.3863648	-1.9282944
C	1.1987358	-0.6926056	-1.9302227
C	1.1987358	0.6926056	-1.9302227

C	0.0000000	1.3863648	-1.9282944
C	-1.1987358	0.6926056	-1.9302227
C	-1.1987358	-0.6926056	-1.9302227
Pt	0.0000000	0.0000000	1.4214731
F	2.3445591	-1.3559058	-1.9180195
F	2.3445591	1.3559058	-1.9180195
F	-2.3445591	1.3559058	-1.9180195
F	-2.3445591	-1.3559058	-1.9180195
F	0.0000000	-2.7075857	-1.9143160
F	0.0000000	2.7075857	-1.9143160

**23a.**

C	2.5048640	1.2072568	-3.2149885
H	3.0885378	2.1354869	-3.2128066
C	3.1918916	0.0000000	-3.2162865
H	4.2723375	0.0000000	-3.2085708
C	2.5048640	-1.2072568	-3.2149885
H	3.0885378	-2.1354869	-3.2128066
O	1.2568339	1.3674200	-3.2163552
O	1.2568339	-1.3674200	-3.2163552
C	-2.5048640	-1.2072568	-3.2149885
H	-3.0885378	-2.1354869	-3.2128066
C	-3.1918916	0.0000000	-3.2162865
H	-4.2723375	0.0000000	-3.2085708
C	-2.5048640	1.2072568	-3.2149885
H	-3.0885378	2.1354869	-3.2128066
O	-1.2568339	-1.3674200	-3.2163552
O	-1.2568339	1.3674200	-3.2163552
C	2.5079274	1.2081248	0.5155403
H	3.0945542	2.1348148	0.5280635
C	3.1921410	0.0000000	0.5715135
H	4.2715971	0.0000000	0.6219630
C	2.5079274	-1.2081248	0.5155403
H	3.0945542	-2.1348148	0.5280635
O	1.2631091	1.3706180	0.4454349

O	1.2631091	-1.3706180	0.4454349
C	-2.5079274	-1.2081248	0.5155403
H	-3.0945542	-2.1348148	0.5280635
C	-3.1921410	0.0000000	0.5715135
H	-4.2715971	0.0000000	0.6219630
C	-2.5079274	1.2081248	0.5155403
H	-3.0945542	2.1348148	0.5280635
O	-1.2631091	-1.3706180	0.4454349
O	-1.2631091	1.3706180	0.4454349
C	0.6936974	1.2016807	3.8270813
C	-0.6936974	1.2016807	3.8270813
C	-1.3875572	0.0000000	3.8318595
C	-0.6936974	-1.2016807	3.8270813
C	0.6936974	-1.2016807	3.8270813
C	1.3875572	0.0000000	3.8318595
H	1.2344040	2.1408801	3.8086689
H	-1.2344040	2.1408801	3.8086689
H	-1.2344040	-2.1408801	3.8086689
H	1.2344040	-2.1408801	3.8086689
H	2.4713290	0.0000000	3.8204256
H	-2.4713290	0.0000000	3.8204256
Ni	0.0000000	0.0000000	0.4457904
Ni	0.0000000	0.0000000	-3.2101530

**23b.**

C	2.5043779	1.2073035	-3.2417003
H	3.0881924	2.1353953	-3.2339079
C	3.1912241	-0.0000000	-3.2243057
H	4.2713238	0.0000000	-3.1945451
C	2.5043779	-1.2073035	-3.2417003
H	3.0881924	-2.1353953	-3.2339079
O	1.2565962	1.3674205	-3.2685214
O	1.2565962	-1.3674205	-3.2685214
C	-2.5043779	-1.2073035	-3.2417003
H	-3.0881924	-2.1353953	-3.2339079



C	-3.1912241	0.0000000	-3.2243057
H	-4.2713238	0.0000000	-3.1945451
C	-2.5043779	1.2073035	-3.2417003
H	-3.0881924	2.1353953	-3.2339079
O	-1.2565962	-1.3674205	-3.2685214
O	-1.2565962	1.3674205	-3.2685214
Ni	0.0000000	0.0000000	-3.2648053
C	2.5063272	1.2079272	0.5392503
H	3.0924960	2.1346968	0.5628126
C	3.1889186	-0.0000000	0.6153037
H	4.2665414	0.0000000	0.6956873
C	2.5063272	-1.2079272	0.5392503
H	3.0924960	-2.1346968	0.5628126
O	1.2635019	1.3701559	0.4386016
O	1.2635019	-1.3701559	0.4386016
C	-2.5063272	-1.2079272	0.5392503
H	-3.0924960	-2.1346968	0.5628126
C	-3.1889186	0.0000000	0.6153037
H	-4.2665414	-0.0000000	0.6956873
C	-2.5063272	1.2079272	0.5392503
H	-3.0924960	2.1346968	0.5628126
O	-1.2635019	-1.3701559	0.4386016
O	-1.2635019	1.3701559	0.4386016
Ni	0.0000000	0.0000000	0.4345900
C	1.2009765	-0.6936994	3.8308508
C	1.2009765	0.6936994	3.8308508
C	0.0000000	1.3882917	3.8275016
C	-1.2009765	0.6936994	3.8308508
C	-1.2009765	-0.6936994	3.8308508
C	0.0000000	-1.3882917	3.8275016
H	2.1404505	-1.2343764	3.8174442
H	2.1404505	1.2343764	3.8174442
H	0.0000000	2.4716292	3.8058057
H	-2.1404505	1.2343764	3.8174442
H	-2.1404505	-1.2343764	3.8174442

H	0.0000000	-2.4716292	3.8058057
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**24a.**

C	2.5050579	1.2070125	-3.2403628
H	3.0883994	2.1353883	-3.2472054
C	3.1916945	0.0000000	-3.2681862
H	4.2719226	0.0000000	-3.2914791
C	2.5050579	-1.2070125	-3.2403628
H	3.0883994	-2.1353883	-3.2472054
O	1.2572773	1.3670226	-3.2052014
O	1.2572773	-1.3670226	-3.2052014
C	-2.5050579	-1.2070125	-3.2403628
H	-3.0883994	-2.1353883	-3.2472054
C	-3.1916945	0.0000000	-3.2681862
H	-4.2719226	0.0000000	-3.2914791
C	-2.5050579	1.2070125	-3.2403628
H	-3.0883994	2.1353883	-3.2472054
O	-1.2572773	-1.3670226	-3.2052014
O	-1.2572773	1.3670226	-3.2052014
C	2.5096549	1.2074134	0.4899191
H	3.0956734	2.1341630	0.4930122
C	3.1948583	-0.0000000	0.4929402
H	4.2751082	0.0000000	0.5014222
C	2.5096549	-1.2074134	0.4899191
H	3.0956734	-2.1341630	0.4930122
O	1.2613919	1.3706119	0.4851698
O	1.2613919	-1.3706119	0.4851698
C	-2.5096549	-1.2074134	0.4899191
H	-3.0956734	-2.1341630	0.4930122
C	-3.1948583	0.0000000	0.4929402
H	-4.2751082	0.0000000	0.5014222
C	-2.5096549	1.2074134	0.4899191
H	-3.0956734	2.1341630	0.4930122
O	-1.2613919	-1.3706119	0.4851698
O	-1.2613919	1.3706119	0.4851698

C	0.6930780	1.2083628	3.8976545
C	-0.6930780	1.2083628	3.8976545
C	-1.3615346	0.0000000	3.9064428
C	-0.6930780	-1.2083628	3.8976545
C	0.6930780	-1.2083628	3.8976545
C	1.3615346	0.0000000	3.9064428
F	2.7024752	0.0000000	3.9125610
F	-2.7024752	0.0000000	3.9125610
Ni	0.0000000	0.0000000	0.4827208
Ni	0.0000000	0.0000000	-3.1957113
H	1.2547783	2.1331652	3.8784111
H	-1.2547783	2.1331652	3.8784111
H	-1.2547783	-2.1331652	3.8784111
H	1.2547783	-2.1331652	3.8784111

**24b.**

C	2.5046013	1.2073291	-3.2041669
H	3.0877745	2.1358271	-3.1975578
C	3.1915296	0.0000000	-3.1889234
H	4.2717441	0.0000000	-3.1653243
C	2.5046013	-1.2073291	-3.2041669
H	3.0877745	-2.1358271	-3.1975578
O	1.2567106	1.3671327	-3.2271457
O	1.2567106	-1.3671327	-3.2271457
C	-2.5046013	-1.2073291	-3.2041669
H	-3.0877745	-2.1358271	-3.1975578
C	-3.1915296	0.0000000	-3.1889234
H	-4.2717441	0.0000000	-3.1653243
C	-2.5046013	1.2073291	-3.2041669
H	-3.0877745	2.1358271	-3.1975578
O	-1.2567106	-1.3671327	-3.2271457
O	-1.2567106	1.3671327	-3.2271457
C	2.5069729	1.2081716	0.5256716
H	3.0918600	2.1356539	0.5446868
C	3.1898834	0.0000000	0.6000171

H	4.2683155	0.0000000	0.6690484
C	2.5069729	-1.2081716	0.5256716
H	3.0918600	-2.1356539	0.5446868
O	1.2632299	1.3692928	0.4314344
O	1.2632299	-1.3692928	0.4314344
C	-2.5069729	-1.2081716	0.5256716
H	-3.0918600	-2.1356539	0.5446868
C	-3.1898834	0.0000000	0.6000171
H	-4.2683155	0.0000000	0.6690484
C	-2.5069729	1.2081716	0.5256716
H	-3.0918600	2.1356539	0.5446868
O	-1.2632299	-1.3692928	0.4314344
O	-1.2632299	1.3692928	0.4314344
C	1.2074749	-0.6931563	3.7955145
C	1.2074749	0.6931563	3.7955145
C	0.0000000	1.3638269	3.7952636
C	-1.2074749	0.6931563	3.7955145
C	-1.2074749	-0.6931563	3.7955145
C	0.0000000	-1.3638269	3.7952636
H	2.1327305	-1.2545386	3.7818885
H	2.1327305	1.2545386	3.7818885
H	-2.1327305	1.2545386	3.7818885
H	-2.1327305	-1.2545386	3.7818885
F	0.0000000	2.7020104	3.7892466
F	0.0000000	-2.7020104	3.7892466
Ni	0.0000000	0.0000000	0.4234622
Ni	0.0000000	0.0000000	-3.2234201

**25a.**

C	2.5047848	1.2073679	-3.1843026
H	3.0880184	2.1358051	-3.1796641
C	3.1917801	0.0000000	-3.1755734
H	4.2721357	0.0000000	-3.1587738
C	2.5047848	-1.2073679	-3.1843026
H	3.0880184	-2.1358051	-3.1796641

O	1.2566733	1.3671458	-3.1983605
O	1.2566733	-1.3671458	-3.1983605
C	-2.5047848	-1.2073679	-3.1843026
H	-3.0880184	-2.1358051	-3.1796641
C	-3.1917801	0.0000000	-3.1755734
H	-4.2721357	0.0000000	-3.1587738
C	-2.5047848	1.2073679	-3.1843026
H	-3.0880184	2.1358051	-3.1796641
O	-1.2566733	-1.3671458	-3.1983605
O	-1.2566733	1.3671458	-3.1983605
C	2.5069454	1.2089528	0.5484509
H	3.0901215	2.1366820	0.5759967
C	3.1891738	0.0000000	0.6213205
H	4.2673533	0.0000000	0.6946487
C	2.5069454	-1.2089528	0.5484509
H	3.0901215	-2.1366820	0.5759967
O	1.2627750	1.3691207	0.4510988
O	1.2627750	-1.3691207	0.4510988
C	-2.5069454	-1.2089528	0.5484509
H	-3.0901215	-2.1366820	0.5759967
C	-3.1891738	0.0000000	0.6213205
H	-4.2673533	-0.0000000	0.6946487
C	-2.5069454	1.2089528	0.5484509
H	-3.0901215	2.1366820	0.5759967
O	-1.2627750	-1.3691207	0.4510988
O	-1.2627750	1.3691207	0.4510988
C	0.6927009	1.1913722	3.7340875
C	-0.6927009	1.1913722	3.7340875
C	-1.3903305	0.0000000	3.7389462
C	-0.6927009	-1.1913722	3.7340875
C	0.6927009	-1.1913722	3.7340875
C	1.3903305	0.0000000	3.7389462
F	-1.3536151	2.3451655	3.7222114
F	1.3536151	2.3451655	3.7222114
F	-1.3536151	-2.3451655	3.7222114

F	1.3536151	-2.3451655	3.7222114
H	-2.4716940	0.0000000	3.7215585
H	-2.4716940	0.0000000	3.7215585
H	2.4716940	0.0000000	3.7215585
Ni	0.0000000	0.0000000	0.4322624
Ni	0.0000000	0.0000000	-3.1945888

**25b.**

C	2.5051465	1.2071514	-3.2025290
H	3.0885688	2.1354816	-3.2035010
C	3.1921212	0.0000000	-3.2136978
H	4.2725748	0.0000000	-3.2175515
C	2.5051465	-1.2071514	-3.2025290
H	3.0885688	-2.1354816	-3.2035010
O	1.2569234	1.3671546	-3.1902638
O	1.2569234	-1.3671546	-3.1902638
C	-2.5051465	-1.2071514	-3.2025290
H	-3.0885688	-2.1354816	-3.2035010
C	-3.1921212	0.0000000	-3.2136978
H	-4.2725748	0.0000000	-3.2175515
C	-2.5051465	1.2071514	-3.2025290
H	-3.0885688	2.1354816	-3.2035010
O	-1.2569234	-1.3671546	-3.1902638
O	-1.2569234	1.3671546	-3.1902638
C	2.5098695	1.2079139	0.5316663
H	3.0945482	2.1346327	0.5545559
C	3.1935173	0.0000000	0.5658905
H	4.2725622	0.0000000	0.6175688
C	2.5098695	-1.2079139	0.5316663
H	3.0945482	-2.1346327	0.5545559
O	1.2619858	1.3706510	0.4787398
O	1.2619858	-1.3706510	0.4787398
C	-2.5098695	-1.2079139	0.5316663
H	-3.0945482	-2.1346327	0.5545559
C	-3.1935173	0.0000000	0.5658905

H	-4.2725622	0.0000000	0.6175688
C	-2.5098695	1.2079139	0.5316663
H	-3.0945482	2.1346327	0.5545559
O	-1.2619858	-1.3706510	0.4787398
O	-1.2619858	1.3706510	0.4787398
C	1.1899604	-0.6927565	3.7876789
C	1.1899604	0.6927565	3.7876789
C	0.0000000	1.3918736	3.7819791
C	-1.1899604	0.6927565	3.7876789
C	-1.1899604	-0.6927565	3.7876789
C	0.0000000	-1.3918736	3.7819791
F	2.3462082	1.3517685	3.7806886
F	2.3462082	-1.3517685	3.7806886
F	-2.3462082	1.3517685	3.7806886
F	-2.3462082	-1.3517685	3.7806886
H	0.0000000	2.4730051	3.7534616
H	0.0000000	-2.4730051	3.7534616
Ni	0.0000000	0.0000000	0.4603744
Ni	0.0000000	0.0000000	-3.1838183

**26a.**

C	2.5051823	1.2070866	-3.2172423
H	3.0882474	2.1355819	-3.2246093
C	3.1918649	0.0000000	-3.2428810
H	4.2721038	0.0000000	-3.2657544
C	2.5051823	-1.2070866	-3.2172423
H	3.0882474	-2.1355819	-3.2246093
O	1.2572098	1.3668432	-3.1836346
O	1.2572098	-1.3668432	-3.1836346
C	-2.5051823	-1.2070866	-3.2172423
H	-3.0882474	-2.1355819	-3.2246093
C	-3.1918649	0.0000000	-3.2428810
H	-4.2721038	0.0000000	-3.2657544
C	-2.5051823	1.2070866	-3.2172423
H	-3.0882474	2.1355819	-3.2246093

O	-1.2572098	-1.3668432	-3.1836346
O	-1.2572098	1.3668432	-3.1836346
C	2.5101509	1.2079315	0.5153443
H	3.0932641	2.1357476	0.5269199
C	3.1948967	0.0000000	0.5176552
H	4.2751007	0.0000000	0.5298257
C	2.5101509	-1.2079315	0.5153443
H	3.0932641	-2.1357476	0.5269199
O	1.2606575	1.3691798	0.5071509
O	1.2606575	-1.3691798	0.5071509
C	-2.5101509	-1.2079315	0.5153443
H	-3.0932641	-2.1357476	0.5269199
C	-3.1948967	-0.0000000	0.5176552
H	-4.2751007	0.0000000	0.5298257
C	-2.5101509	1.2079315	0.5153443
H	-3.0932641	2.1357476	0.5269199
O	-1.2606575	-1.3691798	0.5071509
O	-1.2606575	1.3691798	0.5071509
C	0.6927237	1.2011353	3.8235710
C	-0.6927237	1.2011353	3.8235710
C	-1.3834203	0.0000000	3.8335916
C	-0.6927237	-1.2011353	3.8235710
C	0.6927237	-1.2011353	3.8235710
C	1.3834203	0.0000000	3.8335916
F	-1.3584400	2.3432918	3.8144431
F	1.3584400	2.3432918	3.8144431
F	-1.3584400	-2.3432918	3.8144431
F	1.3584400	-2.3432918	3.8144431
F	2.7068548	0.0000000	3.8464406
F	-2.7068548	0.0000000	3.8464406
Ni	0.0000000	0.0000000	0.4895573
Ni	0.0000000	0.0000000	-3.1750846

**26b.**

C	2.5051911	1.2071560	-3.1988889
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H	3.0882506	2.1356771	-3.2045364
C	3.1920502	0.0000000	-3.2199481
H	4.2723974	0.0000000	-3.2374743
C	2.5051911	-1.2071560	-3.1988889
H	3.0882506	-2.1356771	-3.2045364
O	1.2570947	1.3669135	-3.1716824
O	1.2570947	-1.3669135	-3.1716824
C	-2.5051911	-1.2071560	-3.1988889
H	-3.0882506	-2.1356771	-3.2045364
C	-3.1920502	0.0000000	-3.2199481
H	-4.2723974	-0.0000000	-3.2374743
C	-2.5051911	1.2071560	-3.1988889
H	-3.0882506	2.1356771	-3.2045364
O	-1.2570947	-1.3669135	-3.1716824
O	-1.2570947	1.3669135	-3.1716824
C	2.5101144	1.2081412	0.5356829
H	3.0933652	2.1356174	0.5559412
C	3.1942669	0.0000000	0.5605560
H	4.2738950	0.0000000	0.5985797
C	2.5101144	-1.2081412	0.5356829
H	3.0933652	-2.1356174	0.5559412
O	1.2612855	1.3697099	0.4966595
O	1.2612855	-1.3697099	0.4966595
C	-2.5101144	-1.2081412	0.5356829
H	-3.0933652	-2.1356174	0.5559412
C	-3.1942669	0.0000000	0.5605560
H	-4.2738950	0.0000000	0.5985797
C	-2.5101144	1.2081412	0.5356829
H	-3.0933652	2.1356174	0.5559412
O	-1.2612855	-1.3697099	0.4966595
O	-1.2612855	1.3697099	0.4966595
C	1.1993101	-0.6928397	3.7742725
C	1.1993101	0.6928397	3.7742725
C	-0.0000000	1.3865777	3.7688009
C	-1.1993101	0.6928397	3.7742725

C	-1.1993101	-0.6928397	3.7742725
C	0.0000000	-1.3865777	3.7688009
F	0.0000000	2.7072158	3.7573376
F	0.0000000	-2.7072158	3.7573376
Ni	0.0000000	0.0000000	0.4740850
Ni	0.0000000	0.0000000	-3.1640020
F	2.3440783	1.3569217	3.7711049
F	2.3440783	-1.3569217	3.7711049
F	-2.3440783	1.3569217	3.7711049
F	-2.3440783	-1.3569217	3.7711049

**27a.**

C	2.5843282	1.2288175	-3.2143481
H	3.2117809	2.1282358	-3.2177437
C	3.2369830	0.0000000	-3.2250935
H	4.3182657	0.0000000	-3.2319162
C	2.5843282	-1.2288175	-3.2143481
H	3.2117809	-2.1282358	-3.2177437
O	1.3482830	1.4586747	-3.2001078
O	1.3482830	-1.4586747	-3.2001078
C	-2.5843282	-1.2288175	-3.2143481
H	-3.2117809	-2.1282358	-3.2177437
C	-3.2369830	0.0000000	-3.2250935
H	-4.3182657	0.0000000	-3.2319162
C	-2.5843282	1.2288175	-3.2143481
H	-3.2117809	2.1282358	-3.2177437
O	-1.3482830	-1.4586747	-3.2001078
O	-1.3482830	1.4586747	-3.2001078
C	2.5798010	1.2294116	0.5018256
H	3.2083493	2.1278745	0.5311456
C	3.2297098	0.0000000	0.5589955
H	4.3091213	0.0000000	0.6244777
C	2.5798010	-1.2294116	0.5018256
H	3.2083493	-2.1278745	0.5311456
O	1.3478589	1.4604427	0.4169816

O	1.3478589	-1.4604427	0.4169816
C	-2.5798010	-1.2294116	0.5018256
H	-3.2083493	-2.1278745	0.5311456
C	-3.2297098	0.0000000	0.5589955
H	-4.3091213	0.0000000	0.6244777
C	-2.5798010	1.2294116	0.5018256
H	-3.2083493	2.1278745	0.5311456
O	-1.3478589	-1.4604427	0.4169816
O	-1.3478589	1.4604427	0.4169816
C	0.6937346	1.2018198	3.8447163
C	-0.6937346	1.2018198	3.8447163
C	-1.3875066	-0.0000000	3.8483592
C	-0.6937346	-1.2018198	3.8447163
C	0.6937346	-1.2018198	3.8447163
C	1.3875066	0.0000000	3.8483592
H	1.2345305	2.1410779	3.8285684
H	-1.2345305	2.1410779	3.8285684
H	-1.2345305	-2.1410779	3.8285684
H	1.2345305	-2.1410779	3.8285684
H	2.4714194	0.0000000	3.8378834
H	-2.4714194	0.0000000	3.8378834
Pd	-0.0000000	0.0000000	0.3997473
Pd	0.0000000	0.0000000	-3.1893104

**27b.**

C	2.5829323	1.2290764	-3.2139727
H	3.2103683	2.1284757	-3.2170313
C	3.2352970	0.0000000	-3.2199670
H	4.3165570	0.0000000	-3.2228004
C	2.5829323	-1.2290764	-3.2139727
H	3.2103683	-2.1284757	-3.2170313
O	1.3469737	1.4592965	-3.2053632
O	1.3469737	-1.4592965	-3.2053632
C	-2.5829323	-1.2290764	-3.2139727
H	-3.2103683	-2.1284757	-3.2170313

C	-3.2352970	0.0000000	-3.2199670
H	-4.3165570	0.0000000	-3.2228004
C	-2.5829323	1.2290764	-3.2139727
H	-3.2103683	2.1284757	-3.2170313
O	-1.3469737	-1.4592965	-3.2053632
O	-1.3469737	1.4592965	-3.2053632
C	2.5800701	1.2291627	0.5086318
H	3.2086860	2.1275787	0.5397965
C	3.2294236	-0.0000000	0.5762118
H	4.3081125	-0.0000000	0.6534830
C	2.5800701	-1.2291627	0.5086318
H	3.2086860	-2.1275787	0.5397965
O	1.3490014	1.4598970	0.4103335
O	1.3490014	-1.4598970	0.4103335
C	-2.5800701	-1.2291627	0.5086318
H	-3.2086860	-2.1275787	0.5397965
C	-3.2294236	0.0000000	0.5762118
H	-4.3081125	0.0000000	0.6534830
C	-2.5800701	1.2291627	0.5086318
H	-3.2086860	2.1275787	0.5397965
O	-1.3490014	-1.4598970	0.4103335
O	-1.3490014	1.4598970	0.4103335
C	1.2011176	-0.6937704	3.8367594
C	1.2011176	0.6937704	3.8367594
C	-0.0000000	1.3883020	3.8335088
C	-1.2011176	0.6937704	3.8367594
C	-1.2011176	-0.6937704	3.8367594
C	-0.0000000	-1.3883020	3.8335088
H	2.1405036	-1.2348231	3.8245378
H	2.1405036	1.2348231	3.8245378
H	-0.0000000	2.4717488	3.8136131
H	-2.1405036	1.2348231	3.8245378
H	-2.1405036	-1.2348231	3.8245378
H	-0.0000000	-2.4717488	3.8136131
Pd	0.0000000	0.0000000	0.3919249

Pd	0.0000000	0.0000000	-3.1947902
<b>28a.</b>			
C	2.5832254	1.2287727	-3.2335859
H	3.2103810	2.1282418	-3.2470305
C	3.2352179	0.0000000	-3.2616746
H	4.3161068	0.0000000	-3.2911851
C	2.5832254	-1.2287727	-3.2335859
H	3.2103810	-2.1282418	-3.2470305
O	1.3476502	1.4588016	-3.1923211
O	1.3476502	-1.4588016	-3.1923211
C	-2.5832254	-1.2287727	-3.2335859
H	-3.2103810	-2.1282418	-3.2470305
C	-3.2352179	0.0000000	-3.2616746
H	-4.3161068	0.0000000	-3.2911851
C	-2.5832254	1.2287727	-3.2335859
H	-3.2103810	2.1282418	-3.2470305
O	-1.3476502	-1.4588016	-3.1923211
O	-1.3476502	1.4588016	-3.1923211
C	2.5831476	1.2286376	0.4781666
H	3.2117755	2.1270217	0.4925019
C	3.2342727	0.0000000	0.4917488
H	4.3150013	0.0000000	0.5205815
C	2.5831476	-1.2286376	0.4781666
H	3.2117755	-2.1270217	0.4925019
O	1.3471901	1.4604961	0.4519746
O	1.3471901	-1.4604961	0.4519746
C	-2.5831476	-1.2286376	0.4781666
H	-3.2117755	-2.1270217	0.4925019
C	-3.2342727	0.0000000	0.4917488
H	-4.3150013	0.0000000	0.5205815
C	-2.5831476	1.2286376	0.4781666
H	-3.2117755	2.1270217	0.4925019
O	-1.3471901	-1.4604961	0.4519746
O	-1.3471901	1.4604961	0.4519746
C	0.6931008	1.2085177	3.9052300

C	-0.6931008	1.2085177	3.9052300
C	-1.3613419	0.0000000	3.9115328
C	-0.6931008	-1.2085177	3.9052300
C	0.6931008	-1.2085177	3.9052300
C	1.3613419	0.0000000	3.9115328
F	2.7024877	0.0000000	3.9139492
F	-2.7024877	0.0000000	3.9139492
H	1.2549151	2.1333542	3.8875250
H	-1.2549151	2.1333542	3.8875250
H	-1.2549151	-2.1333542	3.8875250
H	1.2549151	-2.1333542	3.8875250
Pd	0.0000000	0.0000000	0.4374400
Pd	0.0000000	0.0000000	-3.1771874

**28b.**

C	2.5832368	1.2290725	-3.2069641
H	3.2104349	2.1286056	-3.2078123
C	3.2357677	0.0000000	-3.2057751
H	4.3171042	0.0000000	-3.2014787
C	2.5832368	-1.2290725	-3.2069641
H	3.2104349	-2.1286056	-3.2078123
O	1.3471171	1.4590153	-3.2076854
O	1.3471171	-1.4590153	-3.2076854
C	-2.5832368	-1.2290725	-3.2069641
H	-3.2104349	-2.1286056	-3.2078123
C	-3.2357677	0.0000000	-3.2057751
H	-4.3171042	0.0000000	-3.2014787
C	-2.5832368	1.2290725	-3.2069641
H	-3.2104349	2.1286056	-3.2078123
O	-1.3471171	-1.4590153	-3.2076854
O	-1.3471171	1.4590153	-3.2076854
C	2.5796738	1.2292705	0.5135007
H	3.2066545	2.1285624	0.5463498
C	3.2287578	0.0000000	0.5864455
H	4.3071959	0.0000000	0.6666764

C	2.5796738	-1.2292705	0.5135007
H	3.2066545	-2.1285624	0.5463498
O	1.3486255	1.4587684	0.4096324
O	1.3486255	-1.4587684	0.4096324
C	-2.5796738	-1.2292705	0.5135007
H	-3.2066545	-2.1285624	0.5463498
C	-3.2287578	0.0000000	0.5864455
H	-4.3071959	0.0000000	0.6666764
C	-2.5796738	1.2292705	0.5135007
H	-3.2066545	2.1285624	0.5463498
O	-1.3486255	-1.4587684	0.4096324
O	-1.3486255	1.4587684	0.4096324
C	1.2077521	-0.6931765	3.8165309
C	1.2077521	0.6931765	3.8165309
C	-0.0000000	1.3634521	3.8156415
C	-1.2077521	0.6931765	3.8165309
C	-1.2077521	-0.6931765	3.8165309
C	-0.0000000	-1.3634521	3.8156415
H	2.1328393	-1.2550257	3.8043371
H	2.1328393	1.2550257	3.8043371
H	-2.1328393	1.2550257	3.8043371
H	-2.1328393	-1.2550257	3.8043371
F	-0.0000000	2.7017593	3.8085080
F	-0.0000000	-2.7017593	3.8085080
Pd	0.0000000	0.0000000	-3.1985978
Pd	0.0000000	0.0000000	0.3870067

**29a.**

C	2.5831159	1.2291174	-3.1812620
H	3.2102455	2.1286656	-3.1799544
C	3.2355729	0.0000000	-3.1769798
H	4.3168421	0.0000000	-3.1687280
C	2.5831159	-1.2291174	-3.1812620
H	3.2102455	-2.1286656	-3.1799544
O	1.3469772	1.4589832	-3.1869476

O	1.3469772	-1.4589832	-3.1869476
C	-2.5831159	-1.2291174	-3.1812620
H	-3.2102455	-2.1286656	-3.1799544
C	-3.2355729	0.0000000	-3.1769798
H	-4.3168421	0.0000000	-3.1687280
C	-2.5831159	1.2291174	-3.1812620
H	-3.2102455	2.1286656	-3.1799544
O	-1.3469772	-1.4589832	-3.1869476
O	-1.3469772	1.4589832	-3.1869476
C	2.5781632	1.2298608	0.5318893
H	3.2031212	2.1295222	0.5760646
C	3.2255779	0.0000000	0.6141164
H	4.3027800	0.0000000	0.7100278
C	2.5781632	-1.2298608	0.5318893
H	3.2031212	-2.1295222	0.5760646
O	1.3481048	1.4583569	0.4104837
O	1.3481048	-1.4583569	0.4104837
C	-2.5781632	-1.2298608	0.5318893
H	-3.2031212	-2.1295222	0.5760646
C	-3.2255779	0.0000000	0.6141164
H	-4.3027800	0.0000000	0.7100278
C	-2.5781632	1.2298608	0.5318893
H	-3.2031212	2.1295222	0.5760646
O	-1.3481048	-1.4583569	0.4104837
O	-1.3481048	1.4583569	0.4104837
C	0.6927157	1.1912675	3.7519333
C	-0.6927157	1.1912675	3.7519333
C	-1.3905170	0.0000000	3.7561332
C	-0.6927157	-1.1912675	3.7519333
C	0.6927157	-1.1912675	3.7519333
C	1.3905170	0.0000000	3.7561332
F	-1.3534000	2.3453471	3.7410363
F	1.3534000	2.3453471	3.7410363
F	-1.3534000	-2.3453471	3.7410363
F	1.3534000	-2.3453471	3.7410363



H	-2.4719913	0.0000000	3.7399787
H	2.4719913	0.0000000	3.7399787
Pd	0.0000000	0.0000000	0.3773855
Pd	0.0000000	0.0000000	-3.1794554

**29b.**

C	2.5833183	1.2289330	-3.1942001
H	3.2105691	2.1283846	-3.1971572
C	3.2357303	-0.0000000	-3.2026082
H	4.3169847	0.0000000	-3.2071991
C	2.5833183	-1.2289330	-3.1942001
H	3.2105691	-2.1283846	-3.1971572
O	1.3471412	1.4590446	-3.1827438
O	1.3471412	-1.4590446	-3.1827438
C	-2.5833183	-1.2289330	-3.1942001
H	-3.2105691	-2.1283846	-3.1971572
C	-3.2357303	0.0000000	-3.2026082
H	-4.3169847	-0.0000000	-3.2071991
C	-2.5833183	1.2289330	-3.1942001
H	-3.2105691	2.1283846	-3.1971572
O	-1.3471412	-1.4590446	-3.1827438
O	-1.3471412	1.4590446	-3.1827438
C	2.5809863	1.2290068	0.5196568
H	3.2076735	2.1273498	0.5610803
C	3.2294738	0.0000000	0.5746127
H	4.3071252	0.0000000	0.6614730
C	2.5809863	-1.2290068	0.5196568
H	3.2076735	-2.1273498	0.5610803
O	1.3474540	1.4603174	0.4284729
O	1.3474540	-1.4603174	0.4284729
C	-2.5809863	-1.2290068	0.5196568
H	-3.2076735	-2.1273498	0.5610803
C	-3.2294738	0.0000000	0.5746127
H	-4.3071252	0.0000000	0.6614730
C	-2.5809863	1.2290068	0.5196568

H	-3.2076735	2.1273498	0.5610803
O	-1.3474540	-1.4603174	0.4284729
O	-1.3474540	1.4603174	0.4284729
C	1.1897563	-0.6927712	3.7905314
C	1.1897563	0.6927712	3.7905314
C	-0.0000000	1.3922243	3.7861024
C	-1.1897563	0.6927712	3.7905314
C	-1.1897563	-0.6927712	3.7905314
C	-0.0000000	-1.3922243	3.7861024
F	2.3464981	1.3512191	3.7826432
F	2.3464981	-1.3512191	3.7826432
F	-2.3464981	1.3512191	3.7826432
F	-2.3464981	-1.3512191	3.7826432
H	0.0000000	2.4734848	3.7596828
H	0.0000000	-2.4734848	3.7596828
Pd	0.0000000	0.0000000	-3.1731125
Pd	0.0000000	0.0000000	0.3958510

**30a.**

C	2.5833558	1.2287651	-3.2187407
H	3.2100073	2.1284750	-3.2350747
C	3.2353044	0.0000000	-3.2507758
H	4.3159446	0.0000000	-3.2883192
C	2.5833558	-1.2287651	-3.2187407
H	3.2100073	-2.1284750	-3.2350747
O	1.3478847	1.4584517	-3.1704362
O	1.3478847	-1.4584517	-3.1704362
C	-2.5833558	-1.2287651	-3.2187407
H	-3.2100073	-2.1284750	-3.2350747
C	-3.2353044	0.0000000	-3.2507758
H	-4.3159446	0.0000000	-3.2883192
C	-2.5833558	1.2287651	-3.2187407
H	-3.2100073	2.1284750	-3.2350747
O	-1.3478847	-1.4584517	-3.1704362
O	-1.3478847	1.4584517	-3.1704362

C	2.5825751	1.2291198	0.5051060
H	3.2084823	2.1285768	0.5291493
C	3.2331998	0.0000000	0.5253415
H	4.3135272	-0.0000000	0.5658471
C	2.5825751	-1.2291198	0.5051060
H	3.2084823	-2.1285768	0.5291493
O	1.3459011	1.4592773	0.4663706
O	1.3459011	-1.4592773	0.4663706
C	-2.5825751	-1.2291198	0.5051060
H	-3.2084823	-2.1285768	0.5291493
C	-3.2331998	0.0000000	0.5253415
H	-4.3135272	-0.0000000	0.5658471
C	-2.5825751	1.2291198	0.5051060
H	-3.2084823	2.1285768	0.5291493
O	-1.3459011	-1.4592773	0.4663706
O	-1.3459011	1.4592773	0.4663706
C	0.6927118	1.2010428	3.8406209
C	-0.6927118	1.2010428	3.8406209
C	-1.3834458	0.0000000	3.8491349
C	-0.6927118	-1.2010428	3.8406209
C	0.6927118	-1.2010428	3.8406209
C	1.3834458	-0.0000000	3.8491349
F	-1.3584064	2.3433478	3.8314937
F	1.3584064	2.3433478	3.8314937
F	-1.3584064	-2.3433478	3.8314937
F	1.3584064	-2.3433478	3.8314937
F	2.7070225	-0.0000000	3.8592913
F	-2.7070225	0.0000000	3.8592913
Pd	0.0000000	0.0000000	-3.1552529
Pd	0.0000000	0.0000000	0.4402582

**30b.**

C	2.5835088	1.2289386	-3.2056291
H	3.2105876	2.1284527	-3.2139525
C	3.2358981	0.0000000	-3.2206271

H	4.3170809	-0.0000000	-3.2374744
C	2.5835088	-1.2289386	-3.2056291
H	3.2105876	-2.1284527	-3.2139525
O	1.3473842	1.4587221	-3.1825209
O	1.3473842	-1.4587221	-3.1825209
C	-2.5835088	-1.2289386	-3.2056291
H	-3.2105876	-2.1284527	-3.2139525
C	-3.2358981	0.0000000	-3.2206271
H	-4.3170809	0.0000000	-3.2374744
C	-2.5835088	1.2289386	-3.2056291
H	-3.2105876	2.1284527	-3.2139525
O	-1.3473842	-1.4587221	-3.1825209
O	-1.3473842	1.4587221	-3.1825209
C	2.5813080	1.2291275	0.5317526
H	3.2064611	2.1284469	0.5704016
C	3.2304749	-0.0000000	0.5817878
H	4.3088249	0.0000000	0.6589686
C	2.5813080	-1.2291275	0.5317526
H	3.2064611	-2.1284469	0.5704016
O	1.3467878	1.4592890	0.4501956
O	1.3467878	-1.4592890	0.4501956
C	-2.5813080	-1.2291275	0.5317526
H	-3.2064611	-2.1284469	0.5704016
C	-3.2304749	0.0000000	0.5817878
H	-4.3088249	-0.0000000	0.6589686
C	-2.5813080	1.2291275	0.5317526
H	-3.2064611	2.1284469	0.5704016
O	-1.3467878	-1.4592890	0.4501956
O	-1.3467878	1.4592890	0.4501956
C	1.1992601	-0.6928591	3.7864356
C	1.1992601	0.6928591	3.7864356
C	0.0000000	1.3864926	3.7830735
C	-1.1992601	0.6928591	3.7864356
C	-1.1992601	-0.6928591	3.7864356
C	0.0000000	-1.3864926	3.7830735

F	-0.0000000	2.7073984	3.7741638
F	0.0000000	-2.7073984	3.7741638
F	2.3438976	1.3573401	3.7821538
F	2.3438976	-1.3573401	3.7821538
F	-2.3438976	1.3573401	3.7821538
F	-2.3438976	-1.3573401	3.7821538
Pd	-0.0000000	0.0000000	0.4157268
Pd	0.0000000	0.0000000	-3.1708586

**31a.**

C	2.5784049	1.2322855	-3.2027854
H	3.2035122	2.1310001	-3.2030082
C	3.2229953	0.0000000	-3.2061895
H	4.3045350	0.0000000	-3.2044907
C	2.5784049	-1.2322855	-3.2027854
H	3.2035122	-2.1310001	-3.2030082
O	1.3391162	1.4678199	-3.1990739
O	1.3391162	-1.4678199	-3.1990739
C	-2.5784049	-1.2322855	-3.2027854
H	-3.2035122	-2.1310001	-3.2030082
C	-3.2229953	0.0000000	-3.2061895
H	-4.3045350	0.0000000	-3.2044907
C	-2.5784049	1.2322855	-3.2027854
H	-3.2035122	2.1310001	-3.2030082
O	-1.3391162	-1.4678199	-3.1990739
O	-1.3391162	1.4678199	-3.1990739
C	2.5756999	1.2325000	0.5020722
H	3.2019128	2.1303489	0.5264657
C	3.2185553	-0.0000000	0.5495385
H	4.2986964	0.0000000	0.6055681
C	2.5756999	-1.2325000	0.5020722
H	3.2019128	-2.1303489	0.5264657
O	1.3393795	1.4684881	0.4306794
O	1.3393795	-1.4684881	0.4306794
C	-2.5756999	-1.2325000	0.5020722

H	-3.2019128	-2.1303489	0.5264657
C	-3.2185553	0.0000000	0.5495385
H	-4.2986964	0.0000000	0.6055681
C	-2.5756999	1.2325000	0.5020722
H	-3.2019128	2.1303489	0.5264657
O	-1.3393795	-1.4684881	0.4306794
O	-1.3393795	1.4684881	0.4306794
C	0.6935744	1.2015674	3.8290820
C	-0.6935744	1.2015674	3.8290820
C	-1.3871592	0.0000000	3.8324677
C	-0.6935744	-1.2015674	3.8290820
C	0.6935744	-1.2015674	3.8290820
C	1.3871592	-0.0000000	3.8324677
H	1.2343664	2.1408422	3.8122297
H	-1.2343664	2.1408422	3.8122297
H	-1.2343664	-2.1408422	3.8122297
H	1.2343664	-2.1408422	3.8122297
Pt	0.0000000	0.0000000	0.4139479
Pt	0.0000000	0.0000000	-3.1921356
H	2.4710823	0.0000000	3.8208769
H	-2.4710823	0.0000000	3.8208769

**31b.**

C	2.5772220	1.2322132	-3.2225272
H	3.2002745	2.1320444	-3.2487695
C	3.2213431	0.0000000	-3.2749293
H	4.3016682	-0.0000000	-3.3396900
C	2.5772220	-1.2322132	-3.2225272
H	3.2002745	-2.1320444	-3.2487695
O	1.3401430	1.4665533	-3.1398580
O	1.3401430	-1.4665533	-3.1398580
C	-2.5772220	-1.2322132	-3.2225272
H	-3.2002745	-2.1320444	-3.2487695
C	-3.2213431	0.0000000	-3.2749293
H	-4.3016682	0.0000000	-3.3396900

C	-2.5772220	1.2322132	-3.2225272
H	-3.2002745	2.1320444	-3.2487695
O	-1.3401430	-1.4665533	-3.1398580
O	-1.3401430	1.4665533	-3.1398580
C	2.5755477	1.2331795	0.5008454
H	3.2035583	2.1304491	0.5066124
C	3.2190587	0.0000000	0.5200403
H	4.2998585	0.0000000	0.5359530
C	2.5755477	-1.2331795	0.5008454
H	3.2035583	-2.1304491	0.5066124
O	1.3378484	1.4703204	0.4743814
O	1.3378484	-1.4703204	0.4743814
C	-2.5755477	-1.2331795	0.5008454
H	-3.2035583	-2.1304491	0.5066124
C	-3.2190587	0.0000000	0.5200403
H	-4.2998585	0.0000000	0.5359530
C	-2.5755477	1.2331795	0.5008454
H	-3.2035583	2.1304491	0.5066124
O	-1.3378484	-1.4703204	0.4743814
O	-1.3378484	1.4703204	0.4743814
C	1.2006345	-0.6937610	3.8650253
C	1.2006345	0.6937610	3.8650253
C	0.0000000	1.3890918	3.8676799
C	-1.2006345	0.6937610	3.8650253
C	-1.2006345	-0.6937610	3.8650253
C	0.0000000	-1.3890918	3.8676799
H	2.1417430	-1.2320782	3.8512445
H	2.1417430	1.2320782	3.8512445
H	0.0000000	2.4728816	3.8449091
H	-2.1417430	1.2320782	3.8512445
H	-2.1417430	-1.2320782	3.8512445
H	0.0000000	-2.4728816	3.8449091
Pt	0.0000000	0.0000000	-3.1223050
Pt	-0.0000000	0.0000000	0.4665622

**32a.**

C	2.5791632	1.2320386	-3.2157937
H	3.2040071	2.1308698	-3.2223672
C	3.2237301	0.0000000	-3.2308507
H	4.3051604	0.0000000	-3.2440113
C	2.5791632	-1.2320386	-3.2157937
H	3.2040071	-2.1308698	-3.2223672
O	1.3398436	1.4674208	-3.1940883
O	1.3398436	-1.4674208	-3.1940883
C	-2.5791632	-1.2320386	-3.2157937
H	-3.2040071	-2.1308698	-3.2223672
C	-3.2237301	-0.0000000	-3.2308507
H	-4.3051604	0.0000000	-3.2440113
C	-2.5791632	1.2320386	-3.2157937
H	-3.2040071	2.1308698	-3.2223672
O	-1.3398436	-1.4674208	-3.1940883
O	-1.3398436	1.4674208	-3.1940883
C	2.5775153	1.2318617	0.4800749
H	3.2036365	2.1295921	0.4966851
C	3.2205366	0.0000000	0.4988618
H	4.3011922	0.0000000	0.5358205
C	2.5775153	-1.2318617	0.4800749
H	3.2036365	-2.1295921	0.4966851
O	1.3383810	1.4690984	0.4460094
O	1.3383810	-1.4690984	0.4460094
C	-2.5775153	-1.2318617	0.4800749
H	-3.2036365	-2.1295921	0.4966851
C	-3.2205366	0.0000000	0.4988618
H	-4.3011922	-0.0000000	0.5358205
C	-2.5775153	1.2318617	0.4800749
H	-3.2036365	2.1295921	0.4966851
O	-1.3383810	-1.4690984	0.4460094
O	-1.3383810	1.4690984	0.4460094
C	0.6929358	1.2083134	3.8757411
C	-0.6929358	1.2083134	3.8757411



C	-1.3607845	0.0000000	3.8829138
C	-0.6929358	-1.2083134	3.8757411
C	0.6929358	-1.2083134	3.8757411
C	1.3607845	0.0000000	3.8829138
F	2.7024901	0.0000000	3.8872494
F	-2.7024901	0.0000000	3.8872494
H	1.2548331	2.1330858	3.8566970
H	-1.2548331	2.1330858	3.8566970
H	-1.2548331	-2.1330858	3.8566970
H	1.2548331	-2.1330858	3.8566970
Pt	0.0000000	0.0000000	0.4323626
Pt	0.0000000	0.0000000	-3.1841627

**32b.**

C	2.5788073	1.2322952	-3.2051175
H	3.2035860	2.1311776	-3.2101286
C	3.2235324	-0.0000000	-3.2116430
H	4.3050691	0.0000000	-3.2197122
C	2.5788073	-1.2322952	-3.2051175
H	3.2035860	-2.1311776	-3.2101286
O	1.3394662	1.4675531	-3.1939178
O	1.3394662	-1.4675531	-3.1939178
C	-2.5788073	-1.2322952	-3.2051175
H	-3.2035860	-2.1311776	-3.2101286
C	-3.2235324	-0.0000000	-3.2116430
H	-4.3050691	0.0000000	-3.2197122
C	-2.5788073	1.2322952	-3.2051175
H	-3.2035860	2.1311776	-3.2101286
O	-1.3394662	-1.4675531	-3.1939178
O	-1.3394662	1.4675531	-3.1939178
C	2.5750633	1.2326954	0.5151429
H	3.1998570	2.1313042	0.5418965
C	3.2174770	0.0000000	0.5713961
H	4.2972737	0.0000000	0.6329626
C	2.5750633	-1.2326954	0.5151429

H	3.1998570	-2.1313042	0.5418965
O	1.3390129	1.4677560	0.4336959
O	1.3390129	-1.4677560	0.4336959
C	-2.5750633	-1.2326954	0.5151429
H	-3.1998570	-2.1313042	0.5418965
C	-3.2174770	0.0000000	0.5713961
H	-4.2972737	-0.0000000	0.6329626
C	-2.5750633	1.2326954	0.5151429
H	-3.1998570	2.1313042	0.5418965
O	-1.3390129	-1.4677560	0.4336959
O	-1.3390129	1.4677560	0.4336959
C	1.2075154	-0.6930310	3.8145719
C	1.2075154	0.6930310	3.8145719
C	-0.0000000	1.3630134	3.8129928
C	-1.2075154	0.6930310	3.8145719
C	-1.2075154	-0.6930310	3.8145719
C	-0.0000000	-1.3630134	3.8129928
H	2.1325026	-1.2550874	3.8018785
H	2.1325026	1.2550874	3.8018785
H	-2.1325026	1.2550874	3.8018785
H	-2.1325026	-1.2550874	3.8018785
Pt	0.0000000	0.0000000	-3.1852464
Pt	-0.0000000	0.0000000	0.4141856
F	-0.0000000	2.7017540	3.8034903
F	-0.0000000	-2.7017540	3.8034903

**33a.**

C	2.5782531	1.2323856	-3.1737415
H	3.2030512	2.1312433	-3.1745522
C	3.2227979	0.0000000	-3.1744840
H	4.3043123	0.0000000	-3.1726908
C	2.5782531	-1.2323856	-3.1737415
H	3.2030512	-2.1312433	-3.1745522
O	1.3388479	1.4677213	-3.1719391
O	1.3388479	-1.4677213	-3.1719391

C	-2.5782531	-1.2323856	-3.1737415
H	-3.2030512	-2.1312433	-3.1745522
C	-3.2227979	0.0000000	-3.1744840
H	-4.3043123	0.0000000	-3.1726908
C	-2.5782531	1.2323856	-3.1737415
H	-3.2030512	2.1312433	-3.1745522
O	-1.3388479	-1.4677213	-3.1719391
O	-1.3388479	1.4677213	-3.1719391
C	2.5746492	1.2332555	0.5220714
H	3.1980534	2.1320629	0.5571172
C	3.2158882	0.0000000	0.5847898
H	4.2950492	-0.0000000	0.6581546
C	2.5746492	-1.2332555	0.5220714
H	3.1980534	-2.1320629	0.5571172
O	1.3389412	1.4675699	0.4282469
O	1.3389412	-1.4675699	0.4282469
C	-2.5746492	-1.2332555	0.5220714
H	-3.1980534	-2.1320629	0.5571172
C	-3.2158882	-0.0000000	0.5847898
H	-4.2950492	0.0000000	0.6581546
C	-2.5746492	1.2332555	0.5220714
H	-3.1980534	2.1320629	0.5571172
O	-1.3389412	-1.4675699	0.4282469
O	-1.3389412	1.4675699	0.4282469
C	0.6924797	1.1908338	3.7576648
C	-0.6924797	1.1908338	3.7576648
C	-1.3902516	0.0000000	3.7623951
C	-0.6924797	-1.1908338	3.7576648
C	0.6924797	-1.1908338	3.7576648
C	1.3902516	0.0000000	3.7623951
F	-1.3531860	2.3454783	3.7441673
F	1.3531860	2.3454783	3.7441673
F	-1.3531860	-2.3454783	3.7441673
F	1.3531860	-2.3454783	3.7441673
H	-2.4717183	0.0000000	3.7451173

H	2.4717183	0.0000000	3.7451173
Pt	0.0000000	0.0000000	0.4025047
Pt	0.0000000	0.0000000	-3.1652079

**33b.**

C	2.5785185	1.2322051	-3.1797869
H	3.2034182	2.1309720	-3.1811535
C	3.2230520	0.0000000	-3.1845008
H	4.3045507	0.0000000	-3.1855030
C	2.5785185	-1.2322051	-3.1797869
H	3.2034182	-2.1309720	-3.1811535
O	1.3390783	1.4677258	-3.1733824
O	1.3390783	-1.4677258	-3.1733824
C	-2.5785185	-1.2322051	-3.1797869
H	-3.2034182	-2.1309720	-3.1811535
C	-3.2230520	0.0000000	-3.1845008
H	-4.3045507	0.0000000	-3.1855030
C	-2.5785185	1.2322051	-3.1797869
H	-3.2034182	2.1309720	-3.1811535
O	-1.3390783	-1.4677258	-3.1733824
O	-1.3390783	1.4677258	-3.1733824
C	2.5762722	1.2323353	0.5121585
H	3.2010647	2.1299096	0.5483631
C	3.2172756	0.0000000	0.5584654
H	4.2959214	-0.0000000	0.6335794
C	2.5762722	-1.2323353	0.5121585
H	3.2010647	-2.1299096	0.5483631
O	1.3386862	1.4692471	0.4339915
O	1.3386862	-1.4692471	0.4339915
C	-2.5762722	-1.2323353	0.5121585
H	-3.2010647	-2.1299096	0.5483631
C	-3.2172756	0.0000000	0.5584654
H	-4.2959214	0.0000000	0.6335794
C	-2.5762722	1.2323353	0.5121585
H	-3.2010647	2.1299096	0.5483631

O	-1.3386862	-1.4692471	0.4339915
O	-1.3386862	1.4692471	0.4339915
C	1.1892435	-0.6925304	3.7820625
C	1.1892435	0.6925304	3.7820625
C	0.0000000	1.3920343	3.7789043
C	-1.1892435	0.6925304	3.7820625
C	-1.1892435	-0.6925304	3.7820625
C	0.0000000	-1.3920343	3.7789043
F	2.3466168	1.3510104	3.7716535
F	2.3466168	-1.3510104	3.7716535
F	-2.3466168	1.3510104	3.7716535
F	-2.3466168	-1.3510104	3.7716535
Pt	0.0000000	0.0000000	0.4080108
Pt	0.0000000	0.0000000	-3.1662270
H	0.0000000	2.4732141	3.7503501
H	0.0000000	-2.4732141	3.7503501

**34a.**

C	2.5788406	1.2320716	-3.1932747
H	3.2032395	2.1311054	-3.2042888
C	3.2231524	-0.0000000	-3.2164311
H	4.3042955	0.0000000	-3.2427343
C	2.5788406	-1.2320716	-3.1932747
H	3.2032395	-2.1311054	-3.2042888
O	1.3396928	1.4672263	-3.1584926
O	1.3396928	-1.4672263	-3.1584926
C	-2.5788406	-1.2320716	-3.1932747
H	-3.2032395	-2.1311054	-3.2042888
C	-3.2231524	0.0000000	-3.2164311
H	-4.3042955	0.0000000	-3.2427343
C	-2.5788406	1.2320716	-3.1932747
H	-3.2032395	2.1311054	-3.2042888
O	-1.3396928	-1.4672263	-3.1584926
O	-1.3396928	1.4672263	-3.1584926
C	2.5777155	1.2324733	0.4931069

H	3.2018430	2.1309641	0.5124390
C	3.2202326	0.0000000	0.5099463
H	4.3010134	0.0000000	0.5433301
C	2.5777155	-1.2324733	0.4931069
H	3.2018430	-2.1309641	0.5124390
O	1.3376996	1.4685037	0.4612104
O	1.3376996	-1.4685037	0.4612104
C	-2.5777155	-1.2324733	0.4931069
H	-3.2018430	-2.1309641	0.5124390
C	-3.2202326	0.0000000	0.5099463
H	-4.3010134	0.0000000	0.5433301
C	-2.5777155	1.2324733	0.4931069
H	-3.2018430	2.1309641	0.5124390
O	-1.3376996	-1.4685037	0.4612104
O	-1.3376996	1.4685037	0.4612104
C	0.6924408	1.2006255	3.8234173
C	-0.6924408	1.2006255	3.8234173
C	-1.3828590	0.0000000	3.8319704
C	-0.6924408	-1.2006255	3.8234173
C	0.6924408	-1.2006255	3.8234173
C	1.3828590	0.0000000	3.8319704
F	-1.3583324	2.3433994	3.8097618
F	1.3583324	2.3433994	3.8097618
F	-1.3583324	-2.3433994	3.8097618
F	1.3583324	-2.3433994	3.8097618
Pt	0.0000000	0.0000000	0.4434125
Pt	0.0000000	0.0000000	-3.1468970
F	2.7070139	0.0000000	3.8379026
F	-2.7070139	0.0000000	3.8379026

**34b.**

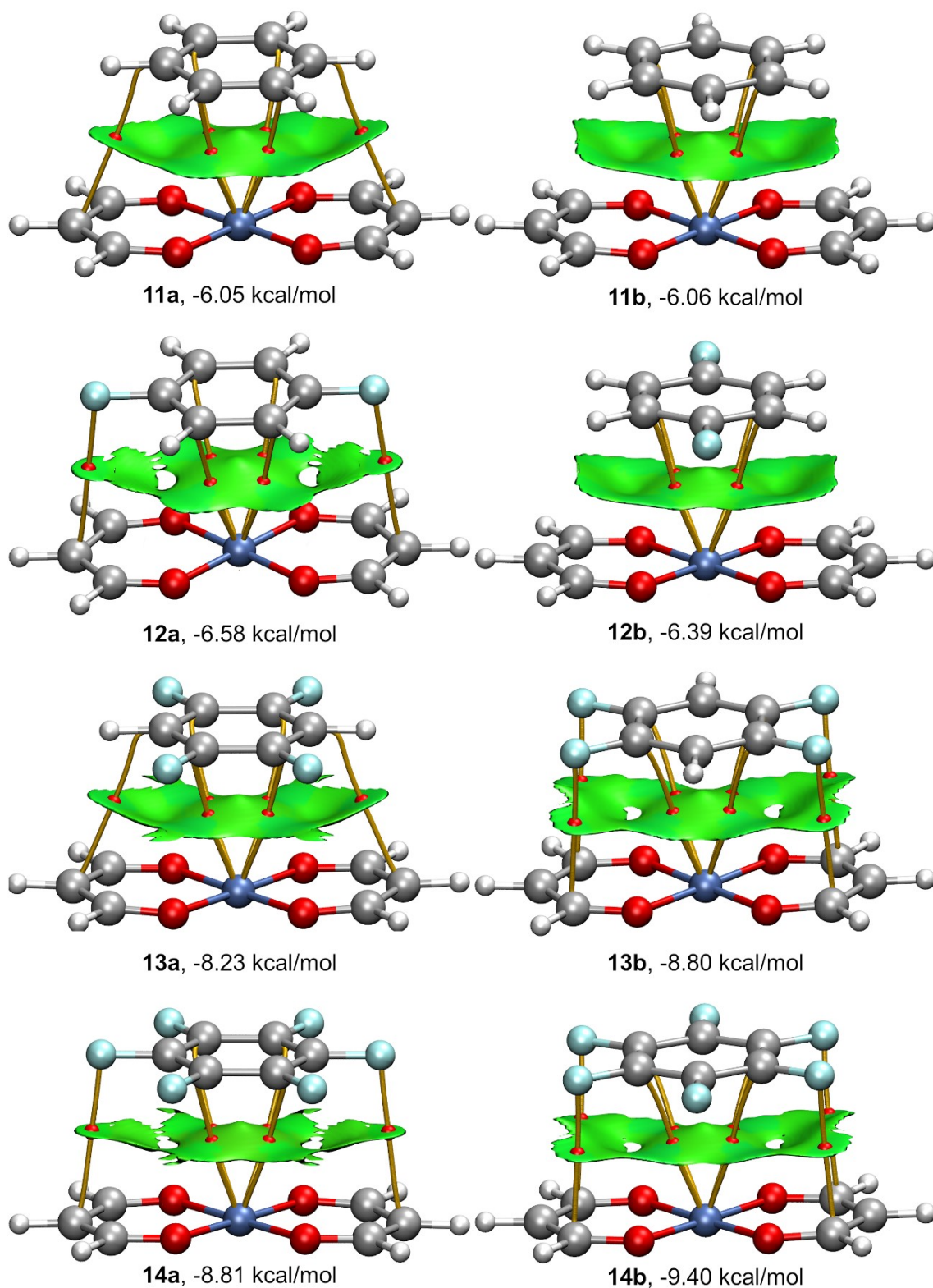
C	2.5785382	1.2322476	-3.1749245
H	3.2033197	2.1310665	-3.1775089
C	3.2229852	0.0000000	-3.1809376
H	4.3044438	0.0000000	-3.1847190

C	2.5785382	-1.2322476	-3.1749245
H	3.2033197	-2.1310665	-3.1775089
O	1.3390493	1.4676487	-3.1659242
O	1.3390493	-1.4676487	-3.1659242
C	-2.5785382	-1.2322476	-3.1749245
H	-3.2033197	-2.1310665	-3.1775089
C	-3.2229852	0.0000000	-3.1809376
H	-4.3044438	0.0000000	-3.1847190
C	-2.5785382	1.2322476	-3.1749245
H	-3.2033197	2.1310665	-3.1775089
O	-1.3390493	-1.4676487	-3.1659242
O	-1.3390493	1.4676487	-3.1659242
C	2.5767439	1.2325100	0.5132150
H	3.2002593	2.1309448	0.5465258
C	3.2181989	-0.0000000	0.5567943
H	4.2974467	0.0000000	0.6239682
C	2.5767439	-1.2325100	0.5132150
H	3.2002593	-2.1309448	0.5465258
O	1.3383921	1.4684620	0.4419740
O	1.3383921	-1.4684620	0.4419740
C	-2.5767439	-1.2325100	0.5132150
H	-3.2002593	-2.1309448	0.5465258
C	-3.2181989	-0.0000000	0.5567943
H	-4.2974467	0.0000000	0.6239682
C	-2.5767439	1.2325100	0.5132150
H	-3.2002593	2.1309448	0.5465258
O	-1.3383921	-1.4684620	0.4419740
O	-1.3383921	1.4684620	0.4419740
C	1.1987001	-0.6925471	3.7713898
C	1.1987001	0.6925471	3.7713898
C	0.0000000	1.3861262	3.7670878
C	-1.1987001	0.6925471	3.7713898
C	-1.1987001	-0.6925471	3.7713898
C	0.0000000	-1.3861262	3.7670878
F	-0.0000000	2.7074248	3.7516005

F	-0.0000000	-2.7074248	3.7516005
F	2.3444582	1.3563126	3.7638233
F	2.3444582	-1.3563126	3.7638233
F	-2.3444582	1.3563126	3.7638233
F	-2.3444582	-1.3563126	3.7638233
Pt	-0.0000000	0.0000000	0.4163594
Pt	0.0000000	0.0000000	-3.1582295

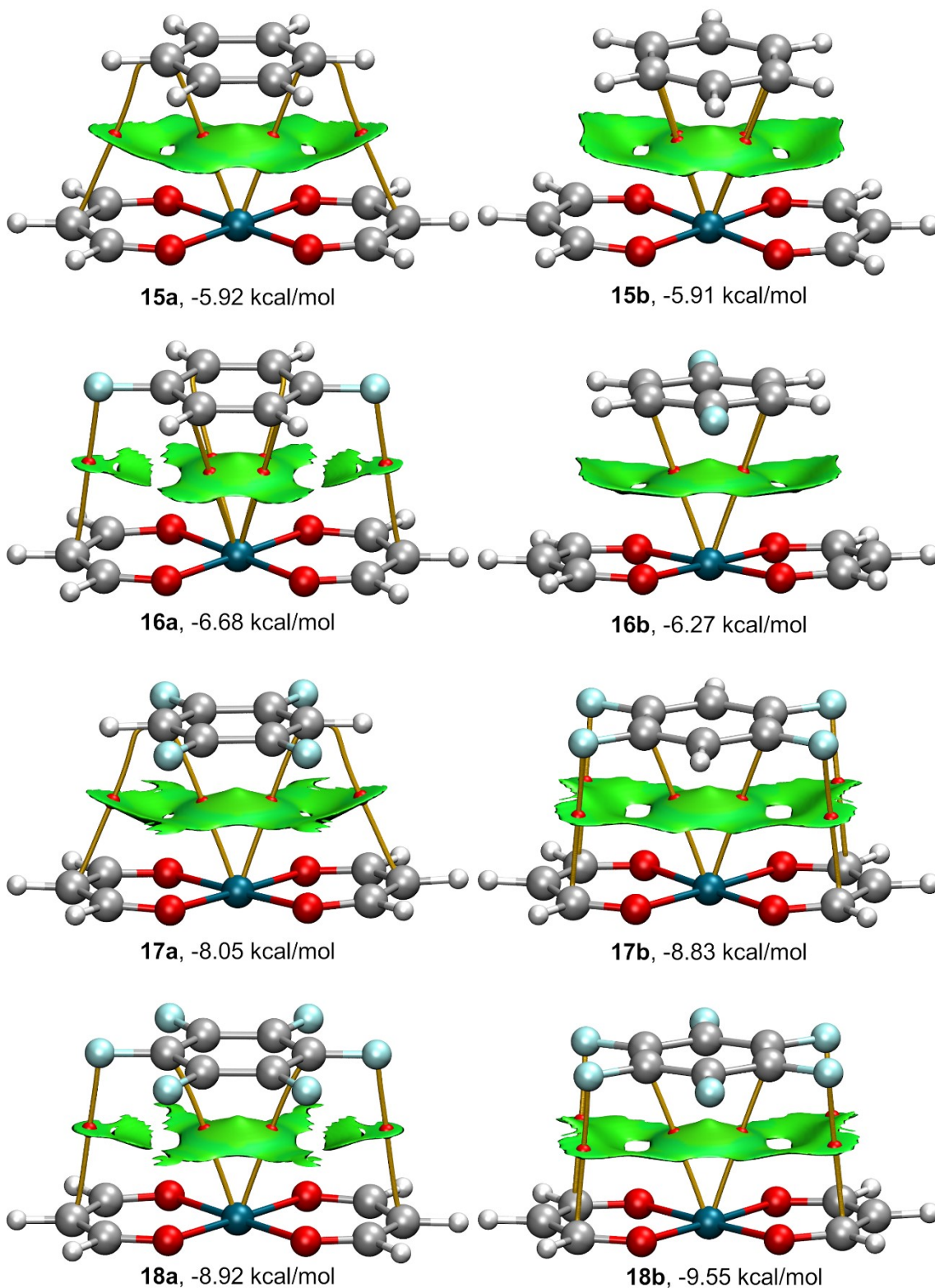


**Figure S1 (QTAIM and NCIplot for nickel complexes 11-14)**



**Figure S1** QTAIM (bond CPs in red and bond paths as solid lines) and NCIplot (RDG = 0.5 a.u.  $\rho$  cut-off = 0.05 a.u., colour range  $\pm 0.035$  a.u.) for nickel complexes **11-14**.

**Figure S2 (QTAIM and NCIplot for palladium complexes 15-18)**



**Figure S2** QTAIM (bond CPs in red and bond paths as solid lines) and NCIplot (RDG = 0.5 a.u.  $\rho$  cut-off = 0.05 a.u., colour range  $\pm 0.035$  a.u.) for palladium complexes **15-18**.

Figure S3 (QTAIM and NCIplot for nickel complexes 23-26)

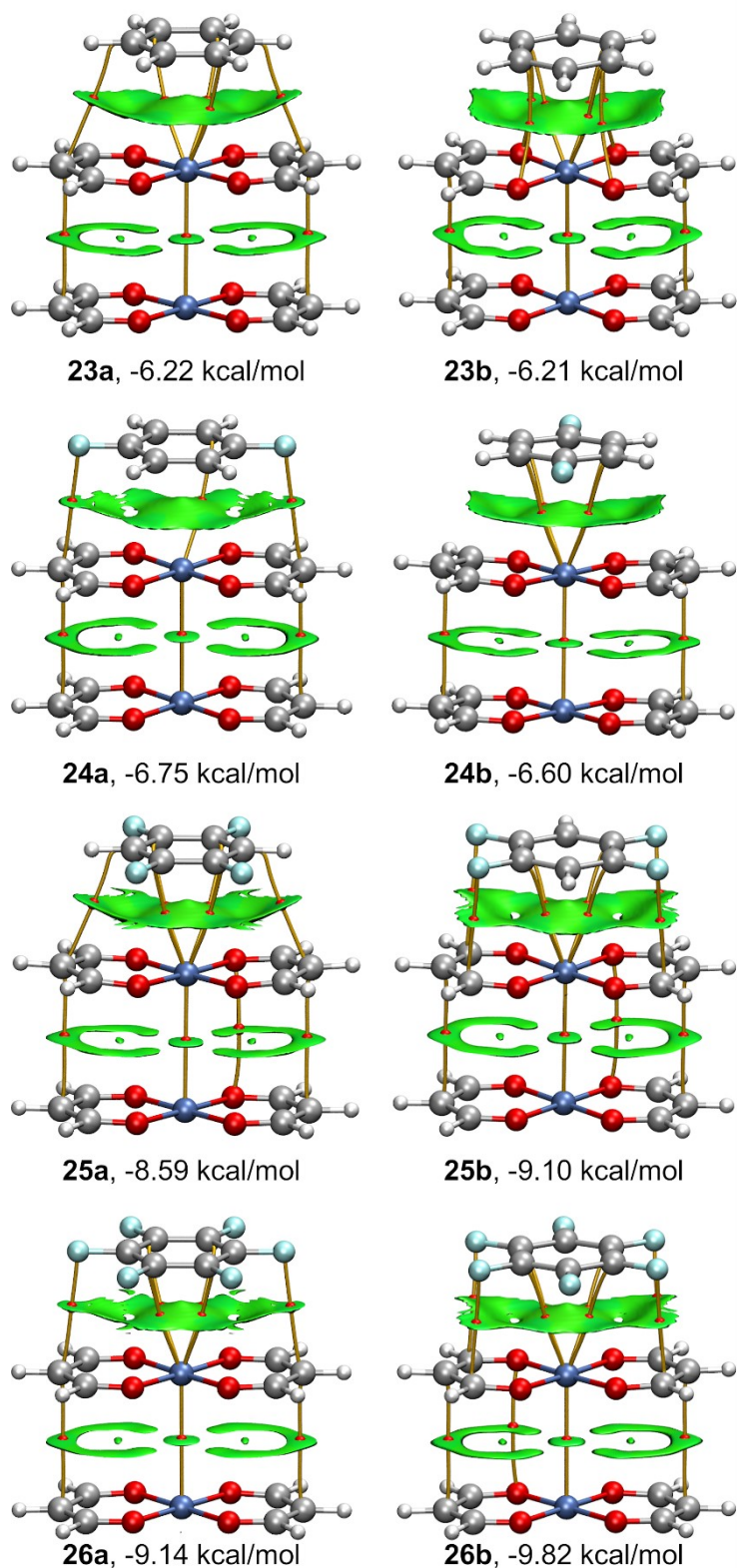


Figure S3 QTAIM (bond CPs in red and bond paths as solid lines) and NCIplot (RDG = 0.5 a.u.  $\rho$  cut-off = 0.05 a.u., colour range  $\pm 0.035$  a.u.) for nickel complexes 23-26.

Figure S4 (QTAIM and NCIplot for palladium complexes 27-30)

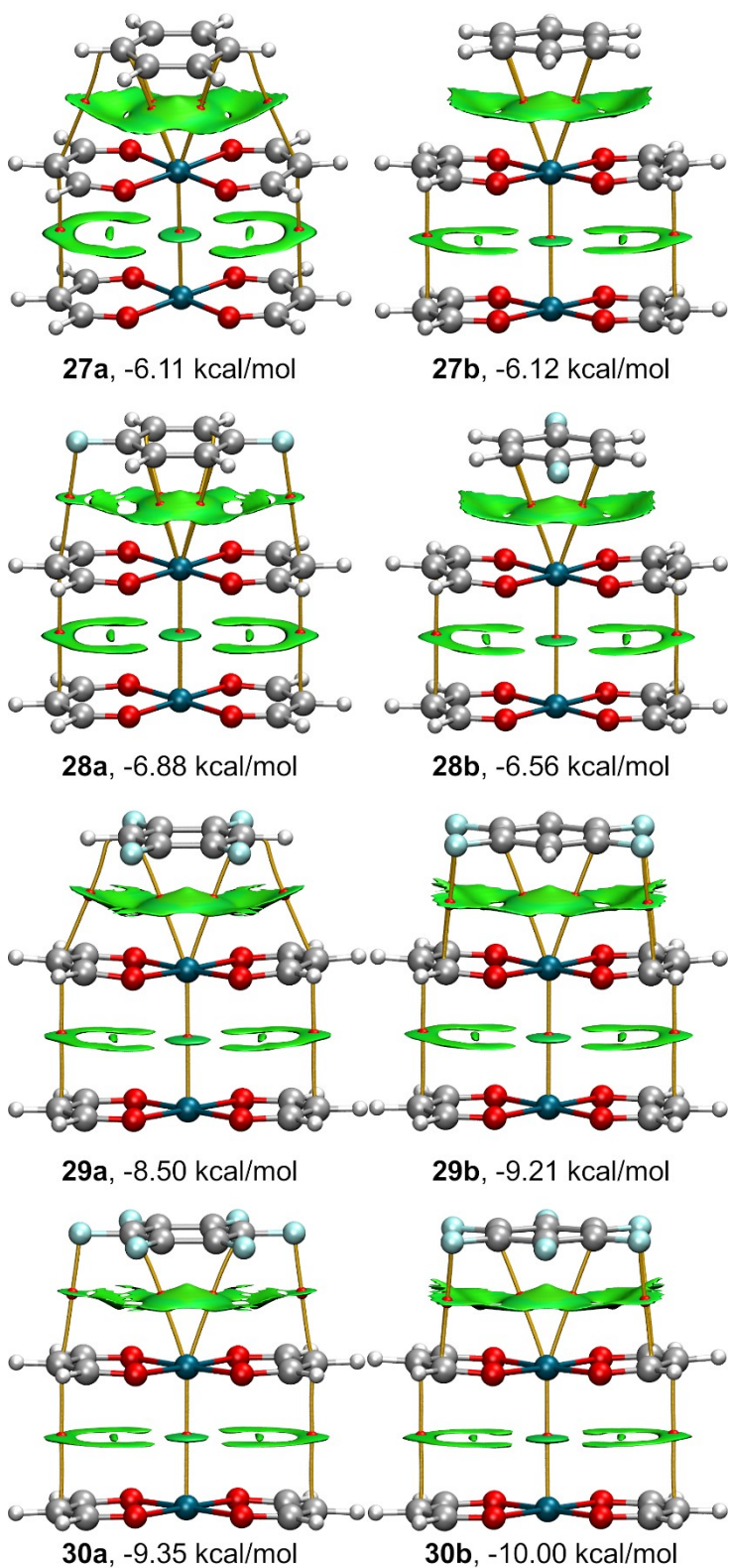


Figure S4 QTAIM (bond CPs in red and bond paths as solid lines) and NCIplot (RDG = 0.5 a.u.  $\rho$  cut-off = 0.05 a.u., colour range  $\pm 0.035$  a.u.) for palladium complexes 27-30.

Figure S5 (QTAIM and NCIplot for platinum complexes 31b-34b)

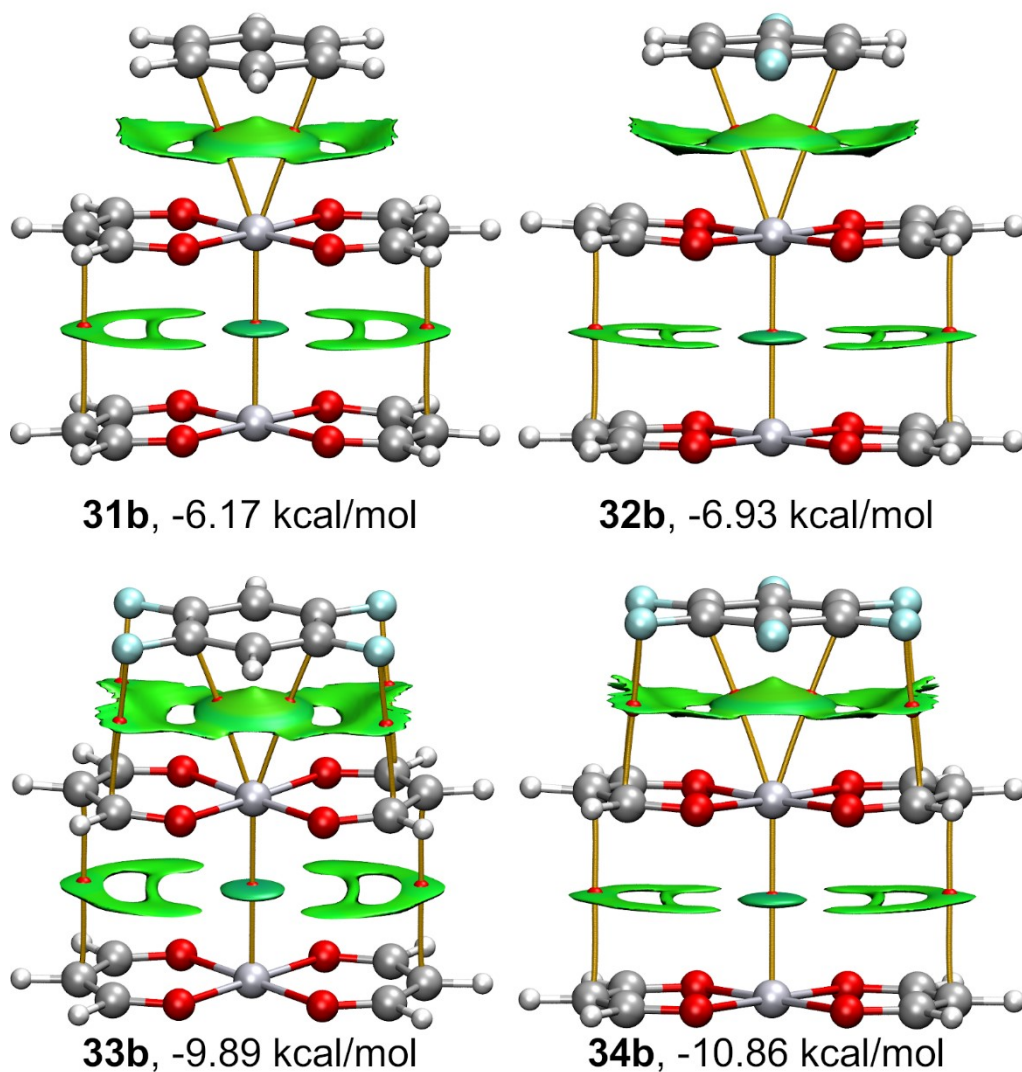


Figure S5 QTAIM (bond CPs in red and bond paths as solid lines) and NCIplot (RDG = 0.5 a.u.  $\rho$  cut-off = 0.05 a.u., colour range  $\pm 0.035$  a.u.) for platinum complexes 31b-34b.