Supporting Information

Effective electronic-only Kohn-Sham equations for the muonic molecules

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Mu-acetylene				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	0.04801	-0.58616	0.00000
Mu	1	-0.94683	-1.20419	0.00000
H	1	0.96878	-1.16584	0.00000
C	6	0.04801	0.71926	0.00000
H	1	-0.66429	1.53126	0.00000

Mu-diazene				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
N	7	0.74076	-0.15096	0.02319
H	1	1.15164	0.78554	-0.03051
N	7	-0.59555	0.02444	-0.06746
H	1	-1.13599	-0.80167	0.14495
Mu	1	-1.07993	0.96698	0.17820

Mu-ethylene				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	-0.69369	0.00000	-0.00200
H	1	-1.10645	-0.88654	-0.49274
H	1	-1.10645	0.88653	-0.49274
Mu	1	-1.12735	0.00000	1.09631
C	6	0.79390	0.00000	-0.01808
H	1	1.35196	0.92631	0.03997
H	1	1.35196	-0.92631	0.03997

Mu-C-formaldehyde				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
O	8	-0.79134	0.00000	0.00732
C	6	0.57435	0.00000	0.01424
H	1	1.00646	0.91035	0.45537
H	1	1.00646	-0.91034	0.45537
Mu	1	0.89218	0.00000	-1.13575

Mu-O-formaldehyde				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	-0.68511	-0.02779	0.05962
H	1	-1.11960	-0.99600	-0.15903
H	1	-1.23591	0.88841	-0.09062
O	8	0.67048	0.12557	-0.02145
Mu	1	1.15299	-0.78134	0.08705

Mu-C-formamide				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
N	7	1.19216	-0.10187	0.00000
H	1	1.35101	-0.67568	0.82140
H	1	1.35101	-0.67567	-0.82141
O	8	-1.21663	-0.37191	0.00000
C	6	-0.13539	0.46225	0.00000
Mu	1	-0.27518	1.18353	-0.93586
H	1	-0.25088	1.13307	0.87248

Mu-O-formamide				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
N	7	-1.12306	-0.25625	-0.04393
H	1	-1.32328	-0.69501	0.85732
H	1	-1.94472	0.22766	-0.38081
C	6	0.04227	0.52813	-0.08608
H	1	0.11354	1.51626	0.36304
O	8	1.21051	-0.17384	0.04520
Mu	1	1.06747	-1.10120	-0.40316

Mu-C-HCN				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	0.00000	0.50241	0.00000
H	1	0.93693	1.07817	0.00000
Mu	1	-1.00799	1.11732	0.00000
N	7	0.00000	-0.73868	0.00000

Mu-N-HCN				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	-0.00030	0.64744	0.00000
H	1	0.89589	1.28025	0.00000
N	7	-0.00030	-0.58320	0.00000
Mu	1	-0.95653	-1.12482	0.00000

Mu-C-methenamine				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
N	7	-0.80316	-0.15310	0.00000
H	1	-1.21222	0.78947	0.00000
C	6	0.62833	0.01211	0.00000
H	1	1.12743	-0.95854	0.00000
H	1	0.96848	0.58405	-0.87858
Mu	1	1.00018	0.61822	0.94259

Mu-N-methenamine				
Atom type	Nuclear charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	-0.72897	0.00000	0.07812
H	1	-1.24362	-0.93097	-0.11838
H	1	-1.24363	0.93097	-0.11839
N	7	0.65504	0.00000	-0.09205
H	1	1.13790	0.83602	0.20621
Mu	1	1.17885	-0.89694	0.20848

exo-Cp-staggered				
Atom	Charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	4.58331	1.34874	0.00087
C	6	4.28455	0.57184	-1.14566
C	6	4.28319	0.56404	1.14185
C	6	3.86885	-0.72852	-0.71811
C	6	3.86834	-0.73332	0.70525
H	1	4.90815	2.37867	0.00460
H	1	4.37397	0.89710	-2.17191
H	1	4.37095	0.88270	2.17031
H	1	3.62205	-1.55676	-1.36540
H	1	3.62040	-1.56562	1.34689
Fe	26	2.43015	0.64833	-0.00339
C	6	1.09284	2.00836	-0.72137
C	6	1.09351	2.01294	0.70742
C	6	0.71950	0.70493	-1.14651
C	6	0.72062	0.71223	1.14128
C	6	0.00000	0.00000	0.00000
H	1	1.39915	2.82811	-1.35629
H	1	1.40042	2.83661	1.33696
H	1	0.62301	0.41484	-2.18441
H	1	0.62498	0.42872	2.18108
Mu	1	-1.11732	0.16641	-0.00004
H	1	0.15567	-1.08243	0.00327

endo-Cp-staggered				
Atom	Charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	4.58959	1.34689	-0.00093
C	6	4.28926	0.56055	-1.14067
C	6	4.29194	0.57174	1.14694
C	6	3.87466	-0.73605	-0.70195
C	6	3.87574	-0.72916	0.72149
H	1	4.91411	2.37691	-0.00633
H	1	4.37660	0.87777	-2.16960
H	1	4.38222	0.89845	2.17265
H	1	3.62743	-1.56946	-1.34247
H	1	3.63051	-1.55672	1.37025
Fe	26	2.43573	0.64653	0.00546
C	6	1.10122	2.01238	-0.70383
C	6	1.09970	2.00581	0.72470
C	6	0.72695	0.71206	-1.13968
C	6	0.72446	0.70162	1.14773
C	6	0.00000	0.00000	0.00000
H	1	1.41047	2.83640	-1.33192
H	1	1.40765	2.82386	1.36116
H	1	0.63355	0.43088	-2.18035
H	1	0.62905	0.41062	2.18552
H	1	-1.09212	0.17558	-0.00036
Mu	1	0.14839	-1.09955	-0.00487

exo-Cp-eclipsed				
Atom	Charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	4.54825	-0.70758	-0.50978
C	6	4.54736	0.70860	-0.50968
C	6	3.99679	-1.14808	0.73334
C	6	3.99536	1.14831	0.73347
C	6	3.68567	-0.00011	1.50973
H	1	4.89490	-1.34612	-1.30860
H	1	4.89328	1.34772	-1.30835
H	1	3.86371	-2.17556	1.03752
H	1	3.86113	2.17549	1.03806
H	1	3.25212	-0.00020	2.49933
Fe	26	2.48866	-0.00043	-0.28915
C	6	1.37178	-0.71599	-1.83149
C	6	1.37217	0.71435	-1.83182
C	6	0.80926	-1.14610	-0.60075
C	6	0.81001	1.14541	-0.60117
C	6	0.00000	0.00000	0.00000
H	1	1.79325	-1.34773	-2.60084
H	1	1.79403	1.34533	-2.60157
H	1	0.66954	-2.18453	-0.33126
H	1	0.67083	2.18412	-0.33246
Mu	1	-1.08406	0.00044	-0.31808
H	1	0.00219	-0.00020	1.09405

endo-Cp-eclipsed				
Atom	Charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	4.55382	-0.70764	-0.50563
C	6	4.55468	0.70865	-0.50594
C	6	4.00353	-1.14713	0.73820
C	6	4.00478	1.14926	0.73777
C	6	3.69465	0.00128	1.51457
H	1	4.89870	-1.34701	-1.30454
H	1	4.90035	1.34704	-1.30529
H	1	3.86964	-2.17414	1.04350
H	1	3.87219	2.17686	1.04183
H	1	3.26296	0.00067	2.50501
Fe	26	2.49499	0.00159	-0.28506
C	6	1.38124	-0.71424	-1.82773
C	6	1.38021	0.71588	-1.82791
C	6	0.81626	-1.14493	-0.59762
C	6	0.81450	1.14602	-0.59798
C	6	0.00000	0.00000	0.00000
H	1	1.80631	-1.34529	-2.59572
H	1	1.80399	1.34777	-2.59596
H	1	0.67950	-2.18398	-0.32889
H	1	0.67555	2.18486	-0.32948
H	1	-1.05768	-0.00098	-0.32393
Mu	1	-0.00786	0.00067	1.11038

Fe-eclipsed				
ATOM	ATOMIC	Coordintes (Angstrom)		
		X	Y	Z
C	6	0.70005	1.65236	1.34099
C	6	-0.70591	1.65216	1.33737
C	6	0.70579	-1.65227	1.33742
C	6	-0.70015	-1.65240	1.34104
C	6	1.15075	1.83060	-0.00339
C	6	-1.14985	1.83073	-0.00920
C	6	1.14971	-1.83085	-0.00917
C	6	-1.15088	-1.83046	-0.00334
C	6	0.00259	2.01276	-0.82814
C	6	-0.00275	-2.01271	-0.82811
H	1	1.33558	1.49178	2.19883
H	1	-1.34558	1.49151	2.19213
H	1	1.34546	-1.49170	2.19219
H	1	-1.33566	-1.49169	2.19887
H	1	-2.17620	1.89495	-0.33733
H	1	2.17867	1.89477	-0.32663
H	1	-2.17880	-1.89438	-0.32660
H	1	2.17607	-1.89527	-0.33728
H	1	0.00522	2.25816	-1.87873
H	1	-0.00537	-2.25805	-1.87871
Fe	26	0.00000	0.00000	0.00000
Mu	1	0.00002	0.00002	-1.52429

Fe-staggered				
Atom	Charge	Coordinates (Angstrom)		
		X	Y	Z
C	6	-1.64609	0.71573	-1.18184
C	6	-0.45784	1.14392	-1.83465
C	6	0.24921	0.00078	-2.28317
C	6	-0.45613	-1.14352	-1.83543
C	6	-1.64489	-0.71775	-1.18208
H	1	-2.42255	1.35442	-0.79080
H	1	-0.15841	2.17187	-1.97759
H	1	1.20444	0.00104	-2.78565
H	1	-0.15491	-2.17089	-1.97872
H	1	-2.42050	-1.35782	-0.79166
Fe	26	0.00000	0.00000	0.00000
C	6	0.65487	0.00016	2.07423
C	6	1.17236	1.15047	1.41057
C	6	2.09538	0.70096	0.41616
C	6	2.09430	-0.70344	0.41629
C	6	1.17068	-1.15121	1.41094
H	1	0.00497	0.00104	2.93531
H	1	0.96449	2.17784	1.66811
H	1	2.64835	1.33730	-0.25853
H	1	2.64628	-1.34093	-0.25811
H	1	0.96103	-2.17815	1.66877
Mu	1	-1.15470	0.00104	0.98778