

Supplementary Information

Tuning Second-Order Nonlinear Optical Response of Organoimido-Substituted Hexamolybdates through Halogens: Quantum Design of Novel Organic-Inorganic Hybrid NLO Material

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Optimized Cartesian Coordinates of Systems 1–6

System 1

Mo	2.269450	2.363819	0.000000
O	2.263619	1.901137	-1.899653
Mo	2.259663	-0.000120	-2.368134
O	2.193963	-0.000186	0.000000
Mo	2.269826	-2.364397	0.000000
O	2.263619	1.901137	1.899653
Mo	2.259663	-0.000120	2.368134
O	0.362747	1.914347	0.000000
Mo	-0.025446	-0.000830	0.000000
O	4.164619	1.895935	0.000000
Mo	4.632743	-0.000431	0.000000
O	2.264074	-1.901351	-1.899625
O	0.365944	-0.000690	-1.938546
O	4.160290	0.000365	-1.889756
O	2.270729	-0.000080	-4.095226
O	2.264074	-1.901351	1.899625
O	0.362885	-1.916633	0.000000
O	4.164888	-1.895359	0.000000
O	2.263090	-4.091010	0.000000
O	0.365944	-0.000690	1.938546

O	4.160290	0.000365	1.889756
O	2.270729	-0.000080	4.095226
O	6.355872	0.000722	0.000000
O	2.264538	4.090585	0.000000
N	-1.837055	-0.001621	0.000000
C	-3.185760	-0.000233	0.000000
C	-3.901774	0.000772	-1.241277
C	-3.901774	0.000772	1.241277
C	-5.288977	0.005226	-1.216322
C	-3.124535	-0.001333	-2.528610
C	-5.288977	0.005226	1.216322
C	-3.124535	-0.001333	2.528610
H	-5.843096	0.005139	-2.157078
C	-6.013984	0.008758	0.000000
H	-2.456278	0.869872	-2.586452
H	-2.461916	-0.876736	-2.587923
H	-3.796604	0.001839	-3.397385
H	-5.843096	0.005139	2.157078
H	-2.461916	-0.876736	2.587923
H	-2.456278	0.869872	2.586452
H	-3.796604	0.001839	3.397385
C	-7.425546	0.014562	0.000000
C	-8.651725	0.018456	0.000000
C	-10.065711	0.012398	0.000000
C	-10.802833	0.003049	1.209130
C	-10.802833	0.003049	-1.209130
C	-12.194451	-0.012428	1.200860
H	-10.259436	0.000276	2.153977
H	-10.259436	0.000276	-2.153977
C	-12.194451	-0.012428	-1.200860
C	-12.923625	-0.017271	0.000000
H	-12.730611	-0.025739	2.153531
H	-12.730611	-0.025739	-2.153531
C	-14.435162	-0.001887	0.000000
H	-14.841145	-0.504829	0.888872
H	-14.828342	1.028022	0.000000
H	-14.841145	-0.504829	-0.888872

System 2

Mo	0.000000	2.363028	2.933695
O	1.899228	1.900795	2.927227
Mo	2.367476	0.000000	2.922348
O	0.000000	0.000000	2.855518
Mo	0.000000	-2.363028	2.933695
O	-1.899228	1.900795	2.927227
Mo	-2.367476	0.000000	2.922348
O	0.000000	1.909972	1.024914
Mo	0.000000	0.000000	0.634952
O	0.000000	1.895754	4.827713
Mo	0.000000	0.000000	5.296944
O	1.899228	-1.900795	2.927227
O	1.935704	0.000000	1.027426
O	1.888991	0.000000	4.822913
O	4.093859	0.000000	2.937577
O	-1.899228	-1.900795	2.927227
O	0.000000	-1.909972	1.024914
O	0.000000	-1.895754	4.827713
O	0.000000	-4.088997	2.931271

O	-1.935704	0.000000	1.027426
O	-1.888991	0.000000	4.822913
O	-4.093859	0.000000	2.937577
O	0.000000	0.000000	7.019423
O	0.000000	4.088997	2.931271
N	0.000000	0.000000	-1.182285
C	0.000000	0.000000	-2.525941
C	1.244062	0.000000	-3.244000
C	-1.244062	0.000000	-3.244000
C	1.219891	0.000000	-4.628822
C	2.532254	0.000000	-2.468988
C	-1.219891	0.000000	-4.628822
C	-2.532254	0.000000	-2.468988
H	2.159587	0.000000	-5.183764
C	0.000000	0.000000	-5.352219
H	2.592244	0.873660	-1.804275
H	2.592244	-0.873660	-1.804275
H	3.398229	0.000000	-3.143859
H	-2.159587	0.000000	-5.183764
H	-2.592244	-0.873660	-1.804275
H	-2.592244	0.873660	-1.804275
H	-3.398229	0.000000	-3.143859
C	0.000000	0.000000	-6.755680
C	0.000000	0.000000	-7.983091
C	0.000000	0.000000	-9.383437
C	-1.197622	0.000000	-10.140500
C	1.197622	0.000000	-10.140500
C	-1.204295	0.000000	-11.529739
C	1.204295	0.000000	-11.529739
C	0.000000	0.000000	-12.236862
F	2.389088	0.000000	-9.497208
F	-2.389088	0.000000	-9.497208
F	-2.378074	0.000000	-12.212325
F	2.378074	0.000000	-12.212325
F	0.000000	0.000000	-13.595303

System 3

Mo	0.000000	2.362918	3.140291
O	1.899137	1.900747	3.133734
Mo	2.367408	0.000000	3.128872
O	0.000000	0.000000	3.061713
Mo	0.000000	-2.362918	3.140291
O	-1.899137	1.900747	3.133734
Mo	-2.367408	0.000000	3.128872
O	0.000000	1.909334	1.231078
Mo	0.000000	0.000000	0.840962
O	0.000000	1.895766	5.034176
Mo	0.000000	0.000000	5.503509
O	1.899137	-1.900747	3.133734
O	1.935414	0.000000	1.233692
O	1.888941	0.000000	5.029362
O	4.093672	0.000000	3.144250
O	-1.899137	-1.900747	3.133734
O	0.000000	-1.909334	1.231078
O	0.000000	-1.895766	5.034176
O	0.000000	-4.088748	3.137994
O	-1.935414	0.000000	1.233692
O	-1.888941	0.000000	5.029362

O	-4.093672	0.000000	3.144250
O	0.000000	0.000000	7.225877
O	0.000000	4.088748	3.137994
N	0.000000	0.000000	-0.977565
C	0.000000	0.000000	-2.320531
C	1.244436	0.000000	-3.039363
C	-1.244436	0.000000	-3.039363
C	1.220192	0.000000	-4.423892
C	2.532221	0.000000	-2.263741
C	-1.220192	0.000000	-4.423892
C	-2.532221	0.000000	-2.263741
H	2.159901	0.000000	-4.978755
C	0.000000	0.000000	-5.148296
H	2.591667	0.873642	-1.598940
H	2.591667	-0.873642	-1.598940
H	3.398635	0.000000	-2.937949
H	-2.159901	0.000000	-4.978755
H	-2.591667	-0.873642	-1.598940
H	-2.591667	0.873642	-1.598940
H	-3.398635	0.000000	-2.937949
C	0.000000	0.000000	-6.550990
C	0.000000	0.000000	-7.779091
C	0.000000	0.000000	-9.177721
C	-1.195793	0.000000	-9.938031
C	1.195793	0.000000	-9.938031
C	-1.199471	0.000000	-11.326081
C	1.199471	0.000000	-11.326081
C	0.000000	0.000000	-12.050761
F	2.387882	0.000000	-9.293359
F	-2.387882	0.000000	-9.293359
F	-2.385505	0.000000	-11.986077
F	2.385505	0.000000	-11.986077
Cl	0.000000	0.000000	-13.792591

System 4

Mo	0.000000	2.362862	3.579558
O	1.899089	1.900773	3.572824
Mo	2.367373	0.000000	3.567926
O	0.000000	0.000000	3.500670
Mo	0.000000	-2.362862	3.579558
O	-1.899089	1.900773	3.572824
Mo	-2.367373	0.000000	3.567926
O	0.000000	1.908824	1.670012
Mo	0.000000	0.000000	1.279905
O	0.000000	1.895777	5.473275
Mo	0.000000	0.000000	5.942703
O	1.899089	-1.900773	3.572824
O	1.935242	0.000000	1.672675
O	1.888856	0.000000	5.468387
O	4.093558	0.000000	3.583523
O	-1.899089	-1.900773	3.572824
O	0.000000	-1.908824	1.670012
O	0.000000	-1.895777	5.473275
O	0.000000	-4.088605	3.577558
O	-1.935242	0.000000	1.672675
O	-1.888856	0.000000	5.468387
O	-4.093558	0.000000	3.583523
O	0.000000	0.000000	7.664971

O	0.000000	4.088605	3.577558
N	0.000000	0.000000	-0.539269
C	0.000000	0.000000	-1.881941
C	1.244550	0.000000	-2.600870
C	-1.244550	0.000000	-2.600870
C	1.220275	0.000000	-3.985288
C	2.532187	0.000000	-1.825011
C	-1.220275	0.000000	-3.985288
C	-2.532187	0.000000	-1.825011
H	2.160183	0.000000	-4.540086
C	0.000000	0.000000	-4.709960
H	2.591372	0.873686	-1.160179
H	2.591372	-0.873686	-1.160179
H	3.398871	0.000000	-2.498904
H	-2.160183	0.000000	-4.540086
H	-2.591372	-0.873686	-1.160179
H	-2.591372	0.873686	-1.160179
H	-3.398871	0.000000	-2.498904
C	0.000000	0.000000	-6.112606
C	0.000000	0.000000	-7.340687
C	0.000000	0.000000	-8.739121
C	-1.196926	0.000000	-9.498767
C	1.196926	0.000000	-9.498767
C	-1.200698	0.000000	-10.886813
C	1.200698	0.000000	-10.886813
C	0.000000	0.000000	-11.607522
F	2.388870	0.000000	-8.853218
F	-2.388870	0.000000	-8.853218
F	-2.388781	0.000000	-11.543890
F	2.388781	0.000000	-11.543890
Br	0.000000	0.000000	-13.513753

System 5

Mo	0.000000	2.362810	4.005891
O	1.899040	1.900800	3.998977
Mo	2.367316	0.000000	3.994052
O	0.000000	0.000000	3.926737
Mo	0.000000	-2.362810	4.005891
O	-1.899040	1.900800	3.998977
Mo	-2.367316	0.000000	3.994052
O	0.000000	1.908421	2.096094
Mo	0.000000	0.000000	1.706020
O	0.000000	1.895764	5.899450
Mo	0.000000	0.000000	6.369020
O	1.899040	-1.900800	3.998977
O	1.935119	0.000000	2.098800
O	1.888745	0.000000	5.894486
O	4.093438	0.000000	4.009851
O	-1.899040	-1.900800	3.998977
O	0.000000	-1.908421	2.096094
O	0.000000	-1.895764	5.899450
O	0.000000	-4.088494	4.004156
O	-1.935119	0.000000	2.098800
O	-1.888745	0.000000	5.894486
O	-4.093438	0.000000	4.009851
O	0.000000	0.000000	8.091246
O	0.000000	4.088494	4.004156
N	0.000000	0.000000	-0.113575

C	0.000000	0.000000	-1.456090
C	1.244834	0.000000	-2.174723
C	-1.244834	0.000000	-2.174723
C	1.220460	0.000000	-3.559071
C	2.532419	0.000000	-1.398546
C	-1.220460	0.000000	-3.559071
C	-2.532419	0.000000	-1.398546
H	2.160205	0.000000	-4.114109
C	0.000000	0.000000	-4.283642
H	2.591772	0.873668	-0.733663
H	2.591772	-0.873668	-0.733663
H	3.399297	0.000000	-2.072310
H	-2.160205	0.000000	-4.114109
H	-2.591772	-0.873668	-0.733663
H	-2.591772	0.873668	-0.733663
H	-3.399297	0.000000	-2.072310
C	0.000000	0.000000	-5.686357
C	0.000000	0.000000	-6.914133
C	0.000000	0.000000	-8.312652
C	-1.196680	0.000000	-9.072710
C	1.196680	0.000000	-9.072710
C	-1.198495	0.000000	-10.461641
C	1.198495	0.000000	-10.461641
C	0.000000	0.000000	-11.185687
F	2.388715	0.000000	-8.425755
F	-2.388715	0.000000	-8.425755
F	-2.390377	0.000000	-11.114409
F	2.390377	0.000000	-11.114409
I	0.000000	0.000000	-13.290490

System 6

Mo	0.000000	2.362585	4.865479
O	1.898721	1.900845	4.857785
Mo	2.367145	0.000000	4.852997
O	0.000000	0.000000	4.784918
Mo	0.000000	-2.362585	4.865479
O	-1.898721	1.900845	4.857785
Mo	-2.367145	0.000000	4.852997
O	0.000000	1.905843	2.954077
Mo	0.000000	0.000000	2.564614
O	0.000000	1.895863	6.758208
Mo	0.000000	0.000000	7.228338
O	1.898721	-1.900845	4.857785
O	1.934346	0.000000	2.957235
O	1.888395	0.000000	6.753062
O	4.092790	0.000000	4.869608
O	-1.898721	-1.900845	4.857785
O	0.000000	-1.905843	2.954077
O	0.000000	-1.895863	6.758208
O	0.000000	-4.087801	4.864342
O	-1.934346	0.000000	2.957235
O	-1.888395	0.000000	6.753062
O	-4.092790	0.000000	4.869608
O	0.000000	0.000000	8.950111
O	0.000000	4.087801	4.864342
N	0.000000	0.000000	0.741643
C	0.000000	0.000000	-0.597778
C	1.246481	0.000000	-1.317302

C	-1.246481	0.000000	-1.317302
C	1.221859	0.000000	-2.700203
C	2.532757	0.000000	-0.539700
C	-1.221859	0.000000	-2.700203
C	-2.532757	0.000000	-0.539700
H	2.161063	0.000000	-3.255764
C	0.000000	0.000000	-3.425422
H	2.590650	0.873621	0.125204
H	2.590650	-0.873621	0.125204
H	3.400459	0.000000	-1.212236
H	-2.161063	0.000000	-3.255764
H	-2.590650	-0.873621	0.125204
H	-2.590650	0.873621	0.125204
H	-3.400459	0.000000	-1.212236
C	0.000000	0.000000	-4.825776
C	0.000000	0.000000	-6.055290
C	0.000000	0.000000	-7.451432
C	-1.192581	0.000000	-8.209033
C	1.192581	0.000000	-8.209033
C	-1.233636	0.000000	-9.609404
C	1.233636	0.000000	-9.609404
C	0.000000	0.000000	-10.316129
F	2.328741	0.000000	-7.478983
F	-2.328741	0.000000	-7.478983
I	0.000000	0.000000	-12.457904
C	-2.568818	0.000000	-10.337995
C	2.568818	0.000000	-10.337995
F	-2.709306	1.100835	-11.144538
F	-2.709306	-1.100835	-11.144538
F	-3.647838	0.000000	-9.520255
F	2.709306	1.100835	-11.144538
F	3.647838	0.000000	-9.520255
F	2.709306	-1.100835	-11.144538

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