Supplementary information

for

Theoretical study on photo-induced process of 1-methyl-3-(N-(1,8-naphtalimidyl)ethyl)imidazolium halide species: an application of constrained density functional theory

Submitted by

Takao Otsuka,[a,*] Masato Sumita,[b,c*] Hironori Izawa,[d] Kenji Morihashi[b]

[a.] *Laboratory for Computational Molecular Design, Computational Biology Research Core, RIKEN Quantitative Biology Center (QBiC), QBiC Building B, 6-2-4 Furuedai, Suita, Osaka 565-0874, Japan*

[b.] *Department of Chemistry, Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1, Tennodai, Tsukuba, Ibaraki 305-8571, Japan*

[c.] *Center for Advanced Intelligence Project, RIKEN AIP-FUJITSU Collaboration Center, RIKEN, Nihonbashi 1-chome Mitsui Building, 15th floor, 1-4-1 Nihonbashi, Chuo-ku,Tokyo, 103-0027, Japan*

[d.] *Graduate School of Engineering, Tottori University, 4-101 Koyama-Minami, Tottori 680-8550, Japan.*

Contents:

1. Constraint values for reproducing vertical excitation energies

Experimental S_{M1} vertical excitation energies can be reproduced by tuning constraint values of CDFT (here, the step of constraint value was used as 0.1). As shown in the Table S1, except for MNEI-F complex, the vertical excitation energies of MNEI-X (X=Cl, Br, I) agree with experimental values (approximately 3.65 eV) by using suitable constraint values. For MNEI-F, we should change the constrain manner in conducting the CDFT calculation. See the next section of this SI.

Table S1. Suitable constraint values and relative energies to S_0 Min (optimized at the conventional DFT level)

	MNEI-F	
	Constrained value	S_{M1} / eV (E_h)
S_0 Min	IM: 0.0	14.34
	F: -1.0	(-1109.5905)
	IM: 0.8	9.70
	F: -1.0	(-1109.7611)
	MNEI-Cl	
	Constrained value	S_{M1}
S_0 Min	IM: 0.0	4.96
	Cl: -1.0	(-1470.3210)
	IM: 0.2	3.49
	Cl: -1.0	(-1470.3751)
	MNEI-Br	
	Constrained value	S_{M1}
S_0 Min	IM: 0.0	4.51
	Br: -1.0	(-3584.0329)
	IM: 0.1	3.75
	Br: -1.0	(-3584.0607)
	MNEI-I	
	Constrained value	S_{M1}
S_0 Min	IM: 0.0	4.11
	I: -1.0	(-7929.0436)
	IM: 0.1	3.36
	I: -1.0	(-7930.0714)

2. Vertical excitation energy of MNEI-F by another CDFT constraint condition

In order to reproduce the S_{M1} vertical excited energy of MNEI-F at the CDFT level, we should use the different constraint manner used in the MNEI-X (X = Cl, Br, I); we need to use the constrain manner that the IM group is combined with F as shown in Figure S1.

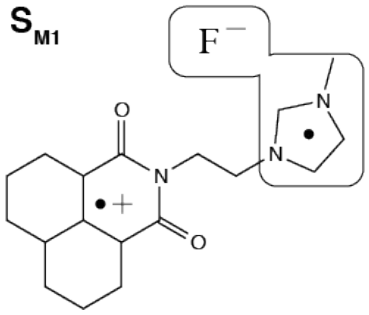

Figure S1. Constrain manner to reproduce the experimental value of the S_{M1} excited energy.

Table S2 shows the vertical excitation energies to the S_{M1} state of MNEI-F using the constraint shown in Figure S1. The vertical excitation energy of MNEI-F by constraint of one negative charge (IM-F: -1.0) is estimated as 6.25 eV. Furthermore, using the suitable constraint value, the vertical excitation energy is optimized to 3.23 eV, which agrees with the experimental value. However, unfortunately, this constraint manner seems to be invalid because the relaxed structure breaks at the CDFT level with this constraint. Therefore, we did not employ this constraint. Careful selection of constraint area is needed to apply CDFT to the excited state.

Table S2. Vertical excited energy to the S_{M1} state on the S_0 Min of MNEI-F

	MNEI-F	
	Constrained value	S_{M1} / eV (E_h)
S_0 Min	IM-F: -1.0	6.25 (-1109.8879)
	IM-F: -0.7	3.23 (-1109.9988)

3. Potential surface of MNEI-F at the DFT and CDFT level

Here we describe the relaxed potential energy surface (PES) of the ground state (S_0) as a function of C3-F bond length with vertical points of the charge separate state (S_{CS}) and the intermolecular ET state (S_{ET}) for MNEI-F. Figure S2 shows the PESs of the S_0, S_{CS}, and S_{ET} state by DFT and CDFT calculations. As shown in Figure S2, S_{ET} state is very close to S_0 state, and the energetic difference between S_0 and S_{ET} states of MNEI-F is relatively small (0.06-1.73 eV). On the other hand, S_{CS} state show the large energetic differences. Therefore, the S_{ET} state of MNEI-F can be regarded as the ground state in the MNEI-F system.

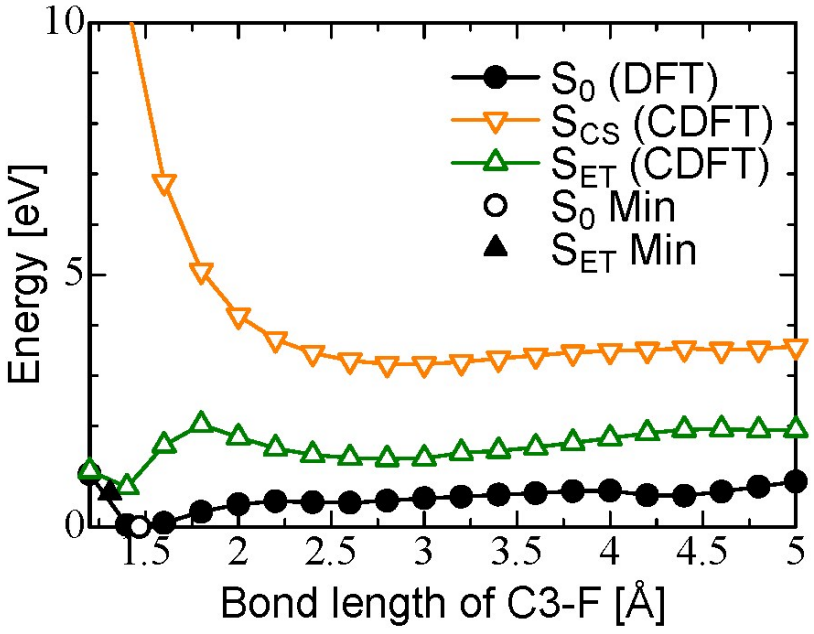

Figure S2. S_0 relaxed potential energy surfaces (PESs) as a function of the C3-F distance with vertical points of S_{CS} and S_{ET} at the conventional DFT and CDFT levels. Energies are shown in the relative values to S_0 Min.

4. Cartesian coordinates at stationary points of each system

4.1 S_0 Min

MNEI-F

C	2.30042439	1.87308563	-1.09490324
C	0.97705237	1.56460867	-0.83317831
C	0.17888476	2.44980166	-0.06678437
C	0.74425940	3.66093445	0.43540961
C	2.10581819	3.94245924	0.14886385
C	2.86577554	3.06671882	-0.59974237
H	2.88833760	1.17882308	-1.68591417
C	-1.17762091	2.14309607	0.20228082
C	-0.08185820	4.52942604	1.19598371
H	2.54283899	4.86264341	0.52900092
H	3.90638762	3.29373937	-0.81179613
C	-1.40173760	4.21157262	1.44528386
C	-1.95417360	3.01331263	0.94699814
H	0.34243042	5.45382230	1.58019898
H	-2.02296307	4.88495679	2.02834498
H	-2.99016530	2.75287941	1.13679365
C	-1.77557553	0.89045856	-0.31704222
C	0.40294952	0.30556035	-1.36672525
N	-0.93847305	0.03921114	-1.05755527
O	1.05906429	-0.46884759	-2.05464133
O	-2.94796320	0.59065377	-0.12824333
C	-1.56125247	-1.19387349	-1.57579204
H	-2.51587150	-0.89860238	-2.01484680
H	-0.90791732	-1.58081916	-2.35700830
C	-1.82900346	-2.26659221	-0.50337806
H	-2.06693290	-1.78150292	0.44977369
H	-2.71976192	-2.82395488	-0.81257572
N	-0.76385270	-3.25742490	-0.35315253
C	-1.03585590	-4.44788129	0.37104422
C	0.54722543	-2.83868480	0.02566728
C	0.10788768	-4.89964736	0.90393891
H	-2.01934721	-4.89329179	0.34827895
H	1.11531032	-2.33613571	-0.75628952

H	0.31775744	-5.81804972	1.43209514
N	1.15018578	-4.01914476	0.53497848
C	2.37960479	-3.90620580	1.29698646
H	2.23661050	-3.41286196	2.26791438
H	2.79116334	-4.90681894	1.46173835
H	3.11043739	-3.33037468	0.72010197
F	0.46775743	-1.80498905	1.06472805

MNEI-Cl

C	2.28169166	1.87078584	-1.07374252
C	0.94759999	1.58885219	-0.83935991
C	0.14149166	2.50432807	-0.11861836
C	0.71305909	3.71779521	0.36889622
C	2.08502096	3.97329381	0.10980721
C	2.85115490	3.06907162	-0.59706925
H	2.87686076	1.14942279	-1.62309151
C	-1.22556392	2.22612692	0.12690741
C	-0.11569484	4.61492396	1.09185754
H	2.52600906	4.89535463	0.48067302
H	3.90073027	3.27457095	-0.78541908
C	-1.44524511	4.32302907	1.32066653
C	-2.00481526	3.12301689	0.83672008
H	0.31557825	5.53961703	1.46759877
H	-2.06692660	5.01668163	1.87893769
H	-3.04731014	2.88016083	1.01362483
C	-1.82934816	0.97529449	-0.37697665
C	0.37130615	0.32628669	-1.34626735
N	-0.99122360	0.10966264	-1.10364022
O	1.02892326	-0.49478920	-1.98460660
O	-3.00620180	0.67860710	-0.20798653
C	-1.61553495	-1.12748072	-1.58708703
H	-2.56709082	-0.84723210	-2.04142911
H	-0.96189854	-1.54430472	-2.35327764
C	-1.91594747	-2.14993222	-0.47481900
H	-2.06236420	-1.63407061	0.47754112
H	-2.83044399	-2.69267898	-0.72888276

N	-0.87780915	-3.16923406	-0.26344707
C	-1.12055492	-4.38728083	0.36472434
C	0.44659249	-2.92832245	-0.21310962
C	0.08092200	-4.91316796	0.70876198
H	-2.12145743	-4.76627973	0.49688225
H	0.94585320	-2.11922315	-0.72013421
H	0.33402007	-5.84325485	1.19229869
N	1.05570946	-4.01796834	0.28835336
C	2.46090937	-4.02095410	0.68129521
H	2.59007003	-3.28138058	1.47886253
H	2.72922553	-5.02120600	1.02562548
H	3.08556189	-3.75675355	-0.17549028
Cl	0.66016538	-1.17006986	1.77129665

MNEI-Br

C	2.10232747	2.02726541	-1.40724711
C	0.80017668	1.75390365	-1.02641669
C	0.08737432	2.67010949	-0.21322782
C	0.72164377	3.87419368	0.21654596
C	2.05746533	4.12148966	-0.19461904
C	2.73147476	3.21772558	-0.99059245
H	2.62650628	1.30529276	-2.02398950
C	-1.24603998	2.40161622	0.18341164
C	-0.01084273	4.77091290	1.03738337
H	2.54532666	5.03676162	0.13151961
H	3.75455746	3.41668111	-1.29534763
C	-1.30822400	4.48777644	1.41420955
C	-1.93075972	3.29777192	0.98596190
H	0.46946697	5.68783437	1.37010824
H	-1.85523068	5.18047140	2.04674483
H	-2.94851717	3.06192294	1.27856376
C	-1.91523125	1.16215575	-0.26100518
C	0.16169700	0.49802980	-1.47013366
N	-1.16799729	0.29309076	-1.07954485
O	0.73969818	-0.33173495	-2.17127792
O	-3.06902946	0.87311132	0.03165210

C	-1.85960240	-0.92675456	-1.51206186
H	-2.85335786	-0.62640724	-1.84688312
H	-1.30371796	-1.33366395	-2.35663471
C	-2.03495925	-1.97102998	-0.39197705
H	-1.99602020	-1.48666157	0.58813921
H	-3.00371543	-2.46345374	-0.50644045
N	-1.02844848	-3.04297255	-0.38387958
C	-1.25402198	-4.31158398	0.13637244
C	0.30154963	-2.85724342	-0.47644216
C	-0.04566935	-4.91321331	0.27723817
H	-2.24932014	-4.66775384	0.34906085
H	0.77715476	-2.00548453	-0.93460321
H	0.21787862	-5.89741052	0.63032266
N	0.91364363	-4.01097198	-0.15841848
C	2.35561121	-4.11568980	0.04235761
H	2.62487631	-3.49440667	0.90365257
H	2.61207260	-5.16167389	0.21836794
H	2.87894979	-3.76142947	-0.84876261
Br	0.85262661	-1.21299002	1.81510148

MNEI-I

C	1.27037490	-2.21222756	2.20407855
C	0.22962907	-1.95635046	1.32781804
C	-0.04871784	-2.85557205	0.26768960
C	0.75269318	-4.02541847	0.10674592
C	1.80890575	-4.25643532	1.02626625
C	2.06079078	-3.36898537	2.05273453
H	1.46723665	-1.50250209	3.00026121
C	-1.10680601	-2.60276924	-0.64031385
C	0.46108667	-4.90493565	-0.96822239
H	2.42323203	-5.14537277	0.90619759
H	2.87598795	-3.55441974	2.74554827
C	-0.57305722	-4.63754079	-1.84257112
C	-1.36184419	-3.48101889	-1.67980279
H	1.07159189	-5.79533234	-1.09682686
H	-0.78060036	-5.31604201	-2.66448395

H	-2.17397826	-3.25674612	-2.36336850
C	-1.94421412	-1.39724832	-0.48296937
C	-0.58198529	-0.73540628	1.50084772
N	-1.63496641	-0.54459616	0.59658012
O	-0.37731786	0.08189140	2.39802711
O	-2.87989603	-1.11770785	-1.22183393
C	-2.49570496	0.63444912	0.74207405
H	-3.52308550	0.29562608	0.60441011
H	-2.37239499	1.00400996	1.75996453
C	-2.21421046	1.73804135	-0.29826007
H	-1.68764703	1.32424122	-1.16463095
H	-3.15779498	2.17281624	-0.63517246
N	-1.40349809	2.85911229	0.20318835
C	-1.50835164	4.16433756	-0.25506952
C	-0.24802267	2.74292059	0.88100927
C	-0.43300977	4.84753850	0.21692134
H	-2.33570480	4.48579765	-0.86733890
H	0.07509047	1.86109118	1.41192224
H	-0.14372973	5.87968699	0.09991268
N	0.32171446	3.95608582	0.96159147
C	1.67440051	4.17928974	1.46508403
H	2.38558141	3.77028081	0.73892428
H	1.82761436	5.25092911	1.60193027
H	1.79502623	3.67148085	2.42405490
I	1.60123245	1.34459482	-1.31046096

4.2 S_{M1} Min

MNEI-F

C	2.34872988	1.72378747	-0.58386573
C	0.97327353	1.51509638	-0.54285573
C	0.10798460	2.53785102	-0.08575580
C	0.65140856	3.78903283	0.32778105
C	2.05547496	3.97134419	0.26558181
C	2.88742036	2.95434950	-0.18054604
H	2.98734103	0.91511640	-0.92066083
C	-1.28570226	2.32128120	-0.01151240

C	-0.23361060	4.78983498	0.79988317
H	2.47758202	4.92079682	0.58481664
H	3.96186513	3.10575785	-0.20797168
C	-1.59953023	4.55767415	0.86300689
C	-2.12810883	3.32088126	0.46157634
H	0.17459530	5.74293409	1.12602007
H	-2.26411653	5.33029149	1.23664776
H	-3.19147198	3.11724976	0.52509656
C	-1.85522699	1.01724744	-0.40691775
C	0.42683745	0.20995902	-0.95705349
N	-0.94914714	0.04805848	-0.89323246
O	1.15974075	-0.68869459	-1.39591974
O	-3.04814719	0.75886137	-0.36248584
C	-1.53363868	-1.24353639	-1.23259948
H	-2.48192887	-1.05274557	-1.73836634
H	-0.86109574	-1.76261343	-1.91581996
C	-1.84651882	-2.11804891	-0.01711618
H	-1.79951197	-1.61891908	0.95570919
H	-2.73138280	-2.74438951	-0.14535350
N	-0.72913351	-3.25936258	0.12796681
C	-0.95264477	-4.58464877	0.41961938
C	0.61001322	-3.06691500	0.08443798
C	0.24509903	-5.23089906	0.53205497
H	-1.95259362	-4.98099873	0.52761875
H	1.07647234	-2.15791586	-0.33756541
H	0.48401051	-6.26400315	0.73477808
N	1.22998479	-4.27927605	0.28087860
C	2.64859758	-4.43920162	0.52289819
H	2.91253897	-4.20561067	1.56396378
H	2.94319385	-5.46905694	0.30148494
H	3.20549416	-3.76633128	-0.13579247
F	-0.28819920	-0.09896891	1.97890755

MNEI-Cl

C	2.23301884	2.02565750	-1.18149980
C	0.91683586	1.71783991	-0.88390027

C	0.12046425	2.63306529	-0.15098540
C	0.68152280	3.87273509	0.28234309
C	2.03521684	4.15330322	-0.04072708
C	2.79257253	3.24902140	-0.75755584
H	2.81964765	1.30740270	-1.74462372
C	-1.22895058	2.32757213	0.15487277
C	-0.14076083	4.76887266	1.01476899
H	2.46833725	5.09573006	0.28581087
H	3.82690636	3.47574648	-0.99906409
C	-1.45303906	4.45109916	1.30168734
C	-2.00182783	3.22540764	0.87037753
H	0.28048129	5.71435229	1.34790132
H	-2.07105797	5.14596872	1.86269017
H	-3.03217220	2.96483802	1.08928646
C	-1.82303734	1.04583572	-0.29395430
C	0.34960520	0.42536964	-1.34058256
N	-0.98930840	0.16830586	-1.00822942
O	1.00892419	-0.38715094	-1.97941307
O	-2.98732253	0.74127011	-0.06764165
C	-1.61299305	-1.08612452	-1.47153559
H	-2.58619994	-0.81094963	-1.88128649
H	-0.98182412	-1.48623875	-2.26390966
C	-1.81677629	-2.14436352	-0.36412464
H	-1.93635743	-1.64485498	0.60675355
H	-2.75630207	-2.66554341	-0.57263765
N	-0.78446547	-3.16643010	-0.32701906
C	-1.07873175	-4.46546838	0.15347100
C	0.56107408	-2.85830214	0.11846698
C	0.06851186	-5.06748877	0.50036404
H	-2.08467850	-4.85695800	0.11410184
H	1.10216391	-2.24258573	-0.60022258
H	0.25158717	-6.08330230	0.81880135
N	1.13658294	-4.17797618	0.25260826
C	2.42313619	-4.33660096	0.89475298
H	2.41297902	-4.06650224	1.96190358
H	2.74001530	-5.37979273	0.79651560

H	3.16545469	-3.70972537	0.38891001
Cl	0.59379166	-1.90173661	1.67940135

MNEI-Br

C	2.17030800	1.90387753	-1.08790139
C	0.81213650	1.71687233	-0.83970704
C	0.05135946	2.73530258	-0.21527390
C	0.68282741	3.95747154	0.15775072
C	2.06323515	4.11823935	-0.11731615
C	2.79265342	3.10691392	-0.72794714
H	2.73034184	1.09868050	-1.54958457
C	-1.31616115	2.53703956	0.07988251
C	-0.09104971	4.94931365	0.80925726
H	2.55261670	5.04483982	0.17098213
H	3.85317142	3.24063773	-0.91521548
C	-1.43387061	4.73623412	1.08663279
C	-2.04819407	3.52739777	0.72785227
H	0.38674183	5.87911107	1.10637571
H	-2.00960153	5.50030924	1.59898320
H	-3.09008978	3.33614110	0.96019059
C	-1.97036426	1.26033203	-0.26722958
C	0.17821842	0.44043929	-1.21622198
N	-1.17293798	0.29262805	-0.92463860
O	0.80608916	-0.44514677	-1.81210387
O	-3.14538708	1.01561328	-0.04238750
C	-1.85000910	-0.95548333	-1.26529598
H	-2.85516593	-0.70125520	-1.60539758
H	-1.30607934	-1.43677733	-2.07848883
C	-2.00438030	-1.91439796	-0.08174306
H	-1.77211691	-1.49652573	0.90344452
H	-2.93248794	-2.48830781	-0.09543443
N	-0.93888624	-3.09767434	-0.20659592
C	-1.15695080	-4.42661810	0.07744901
C	0.38340192	-2.94364549	-0.46489470
C	0.02005415	-5.10871555	-0.03070478
H	-2.13765782	-4.79832709	0.33920251

H	0.80606271	-2.02878259	-0.92052973
H	0.25297429	-6.15459167	0.10070305
N	0.98382085	-4.17977310	-0.41011158
C	2.41805204	-4.38707741	-0.39204541
H	2.84330433	-4.17650512	0.59864632
H	2.63982021	-5.42193297	-0.66693412
H	2.88894305	-3.72214688	-1.12201707
Br	0.16663038	0.03187679	2.44557661

MNEI-I

C	1.89211171	-1.97685044	1.64078677
C	0.59933078	-1.79377290	1.15388284
C	0.01726275	-2.75162518	0.28919859
C	0.76482519	-3.90503106	-0.08800533
C	2.07305698	-4.06481744	0.43145869
C	2.62492667	-3.11624329	1.28185678
H	2.31696668	-1.21660322	2.28655019
C	-1.27799627	-2.55403243	-0.24202977
C	0.17808255	-4.82858610	-0.98776736
H	2.65085503	-4.93854540	0.14218776
H	3.63422957	-3.24678023	1.65840861
C	-1.09573570	-4.61671199	-1.49705495
C	-1.82543144	-3.47767375	-1.12828863
H	0.74790933	-5.70290439	-1.29060562
H	-1.52395439	-5.32571496	-2.19806677
H	-2.81189249	-3.28619736	-1.53595391
C	-2.04346387	-1.34307856	0.10908542
C	-0.14354620	-0.57529985	1.52147341
N	-1.42342760	-0.43045853	0.99387489
O	0.32838835	0.26941285	2.29319918
O	-3.16849031	-1.10295327	-0.30322352
C	-2.21123992	0.75581544	1.32437408
H	-3.23463995	0.43084845	1.52400142
H	-1.79743248	1.20810759	2.22617457
C	-2.28820834	1.77662767	0.19415937
H	-2.00397736	1.41368666	-0.79915806

H	-3.20699219	2.36529150	0.19381446
N	-1.20360357	2.93741444	0.42453475
C	-1.29620530	4.22586664	-0.05825491
C	0.08001566	2.74475807	0.81831058
C	-0.08460703	4.83910333	0.06145192
H	-2.22134168	4.61883170	-0.45672727
H	0.41564335	1.86898963	1.40296572
H	0.23613824	5.83860115	-0.19141567
N	0.77480828	3.91722273	0.64790159
C	2.22382423	4.00168466	0.66894887
H	2.65764726	3.54263875	-0.22887010
H	2.52459737	5.05118831	0.72524612
H	2.60613296	3.47932165	1.55153177
I	0.58290948	0.19870923	-2.34153126

4.3 S_{ET} Min

MNEI-F

C	2.37721504	1.76986156	-0.82086011
C	1.03375248	1.47931340	-0.66238344
C	0.17960169	2.39803188	-0.00320798
C	0.70775202	3.63220490	0.48141748
C	2.09020036	3.89641650	0.29948924
C	2.90685449	2.98283694	-0.33514562
H	3.01057353	1.04698532	-1.32354354
C	-1.19667187	2.11227085	0.16624820
C	-0.17401671	4.54521130	1.11680249
H	2.49794004	4.83427128	0.66924678
H	3.96402953	3.19554146	-0.46450819
C	-1.51300732	4.24708930	1.26761694
C	-2.02785443	3.02311700	0.79374054
H	0.22329219	5.48868604	1.48357244
H	-2.17715979	4.95450237	1.75550432
H	-3.07745390	2.77503646	0.91082554
C	-1.75887938	0.84912296	-0.34974871
C	0.49491723	0.21356027	-1.19908319
N	-0.87224893	-0.01674865	-1.02215031

O	1.19239344	-0.59743079	-1.81294272
O	-2.94474451	0.55352406	-0.26957518
C	-1.47456010	-1.22540413	-1.58653874
H	-2.38640163	-0.91876497	-2.10365284
H	-0.77575792	-1.62839191	-2.32013985
C	-1.90484112	-2.27493898	-0.55519397
H	-2.29479876	-1.77591917	0.33228199
H	-2.69307814	-2.89396153	-0.99619391
N	-0.84685377	-3.19673049	-0.09889701
C	-1.07436934	-4.21881660	0.80362378
C	0.46803505	-3.08661807	-0.29188720
C	0.13715045	-4.72818987	1.15005312
H	-2.06951196	-4.48406729	1.12282608
H	0.95321749	-2.32048649	-0.88691123
H	0.40489473	-5.52493881	1.82550281
N	1.08824153	-4.00850419	0.45124896
C	2.53112428	-4.04798698	0.67928141
H	2.77833601	-3.37816688	1.50640674
H	2.82885334	-5.07253148	0.91212316
H	3.04572482	-3.72115758	-0.22579418
F	0.17594723	-1.05576838	1.73738132

MNEI-Cl

C	2.23301884	2.02565750	-1.18149980
C	0.91683586	1.71783991	-0.88390027
C	0.12046425	2.63306529	-0.15098540
C	0.68152280	3.87273509	0.28234309
C	2.03521684	4.15330322	-0.04072708
C	2.79257253	3.24902140	-0.75755584
H	2.81964765	1.30740270	-1.74462372
C	-1.22895058	2.32757213	0.15487277
C	-0.14076083	4.76887266	1.01476899
H	2.46833725	5.09573006	0.28581087
H	3.82690636	3.47574648	-0.99906409
C	-1.45303906	4.45109916	1.30168734
C	-2.00182783	3.22540764	0.87037753

H	0.28048129	5.71435229	1.34790132
H	-2.07105797	5.14596872	1.86269017
H	-3.03217220	2.96483802	1.08928646
C	-1.82303734	1.04583572	-0.29395430
C	0.34960520	0.42536964	-1.34058256
N	-0.98930840	0.16830586	-1.00822942
O	1.00892419	-0.38715094	-1.97941307
O	-2.98732253	0.74127011	-0.06764165
C	-1.61299305	-1.08612452	-1.47153559
H	-2.58619994	-0.81094963	-1.88128649
H	-0.98182412	-1.48623875	-2.26390966
C	-1.81677629	-2.14436352	-0.36412464
H	-1.93635743	-1.64485498	0.60675355
H	-2.75630207	-2.66554341	-0.57263765
N	-0.78446547	-3.16643010	-0.32701906
C	-1.07873175	-4.46546838	0.15347100
C	0.56107408	-2.85830214	0.11846698
C	0.06851186	-5.06748877	0.50036404
H	-2.08467850	-4.85695800	0.11410184
H	1.10216391	-2.24258573	-0.60022258
H	0.25158717	-6.08330230	0.81880135
N	1.13658294	-4.17797618	0.25260826
C	2.42313619	-4.33660096	0.89475298
H	2.41297902	-4.06650224	1.96190358
H	2.74001530	-5.37979273	0.79651560
H	3.16545469	-3.70972537	0.38891001
Cl	0.59379166	-1.90173661	1.67940135

MNEI-Br

C	2.07259265	2.17034945	-1.41686684
C	0.77680819	1.88126831	-1.02504045
C	0.05226402	2.80325330	-0.22828461
C	0.66304929	4.03195190	0.16759624
C	1.99424162	4.29258551	-0.25144924
C	2.68253805	3.38065507	-1.02594662
H	2.60419582	1.44720241	-2.02639383

C	-1.27372439	2.51462293	0.18015954
C	-0.08854302	4.93690308	0.96215852
H	2.46592971	5.22532175	0.04848886
H	3.70126940	3.59083974	-1.33820234
C	-1.38027730	4.63750149	1.34537310
C	-1.97708745	3.42065287	0.95479484
H	0.37103690	5.87436896	1.26593914
H	-1.94428095	5.33896688	1.95314605
H	-2.99055732	3.17223003	1.25265821
C	-1.91373372	1.23739742	-0.21520500
C	0.15512326	0.60212730	-1.44823112
N	-1.15369440	0.35778045	-1.00344728
O	0.74414190	-0.20829907	-2.15459166
O	-3.05342759	0.93689035	0.11782343
C	-1.81602627	-0.90064811	-1.39405111
H	-2.82548865	-0.63364538	-1.70964718
H	-1.26434845	-1.30419612	-2.24173862
C	-1.89352886	-1.94883863	-0.25647030
H	-1.77875945	-1.44681588	0.71462726
H	-2.89124944	-2.39670544	-0.27058348
N	-0.94785376	-3.03837631	-0.40604773
C	-1.24670683	-4.33868422	0.05928840
C	0.47400232	-2.84064978	-0.20753820
C	-0.10141669	-5.03210929	0.16195629
H	-2.26894896	-4.66087527	0.19301574
H	0.91941378	-2.21891832	-0.98372121
H	0.06202005	-6.07249325	0.40230004
N	0.96351829	-4.19926991	-0.23652318
C	2.33630607	-4.48649799	0.11007756
H	2.57184249	-4.26414623	1.16240117
H	2.53578125	-5.54523240	-0.08345707
H	3.00698868	-3.89510852	-0.52279933
Br	0.90796245	-1.87577227	1.50164083

MNEI-I

C	1.86028929	-2.32551431	1.68793034
C	0.61894752	-2.03667110	1.14821257
C	-0.01063166	-2.96118542	0.27696557
C	0.64057287	-4.19151469	-0.04166244
C	1.91285535	-4.45293043	0.53123938
C	2.50825735	-3.53900895	1.37687177
H	2.31979874	-1.59980041	2.35059589
C	-1.28031413	-2.67376986	-0.28327970
C	-0.01394672	-5.09765217	-0.91688930
H	2.41380598	-5.38787264	0.29240920
H	3.48248447	-3.75041384	1.80757459
C	-1.25123634	-4.79776791	-1.45017760
C	-1.88859796	-3.58000659	-1.13407726
H	0.47687076	-6.03614924	-1.16288291
H	-1.74046690	-5.49981801	-2.11881483
H	-2.85984314	-3.33142993	-1.54900205
C	-1.96267921	-1.39737695	0.03512734
C	-0.04503741	-0.75532276	1.49118736
N	-1.30203742	-0.52119524	0.91204214
O	0.46449802	0.06474126	2.24685385
O	-3.05409949	-1.09363561	-0.42990521
C	-2.00656824	0.73391238	1.22695897
H	-3.04559455	0.46668796	1.42351161
H	-1.55636497	1.13413167	2.13382796
C	-1.94542826	1.78648783	0.08921417
H	-1.60674903	1.30446596	-0.84039314
H	-2.95302410	2.16948870	-0.09234339
N	-1.10745422	2.92331280	0.40416150
C	-1.43361828	4.23765068	0.01787207
C	0.33217584	2.82881242	0.41035584
C	-0.33621359	5.00416801	0.14427441
H	-2.44595813	4.50865194	-0.24237518
H	0.71196757	2.15365187	1.17587068
H	-0.21295025	6.06905457	0.01440029
N	0.71523766	4.19953168	0.61927428

C	2.09973557	4.60004217	0.54613779
H	2.53293359	4.43775565	-0.45346053
H	2.17704242	5.66014882	0.80546962
H	2.69023549	4.02804906	1.27020936
I	1.16858187	1.94853073	-1.50485983

References

S1. T. Otsuka, M. Sumita, H. Izawa, K. Morihasi, Phys. Chem. Chem. Phys., 18, 17795-17798 (2016).