Supporting materials

Towards the best model for hydrogen atoms in experimental charge density refinement

Anna A. Hoser, Paulina M. Dominiak, Krzysztof Woźniak
Chemistry Department, Warsaw University, 02-093 Warszawa, Pasteura 1, Poland.

Abstract

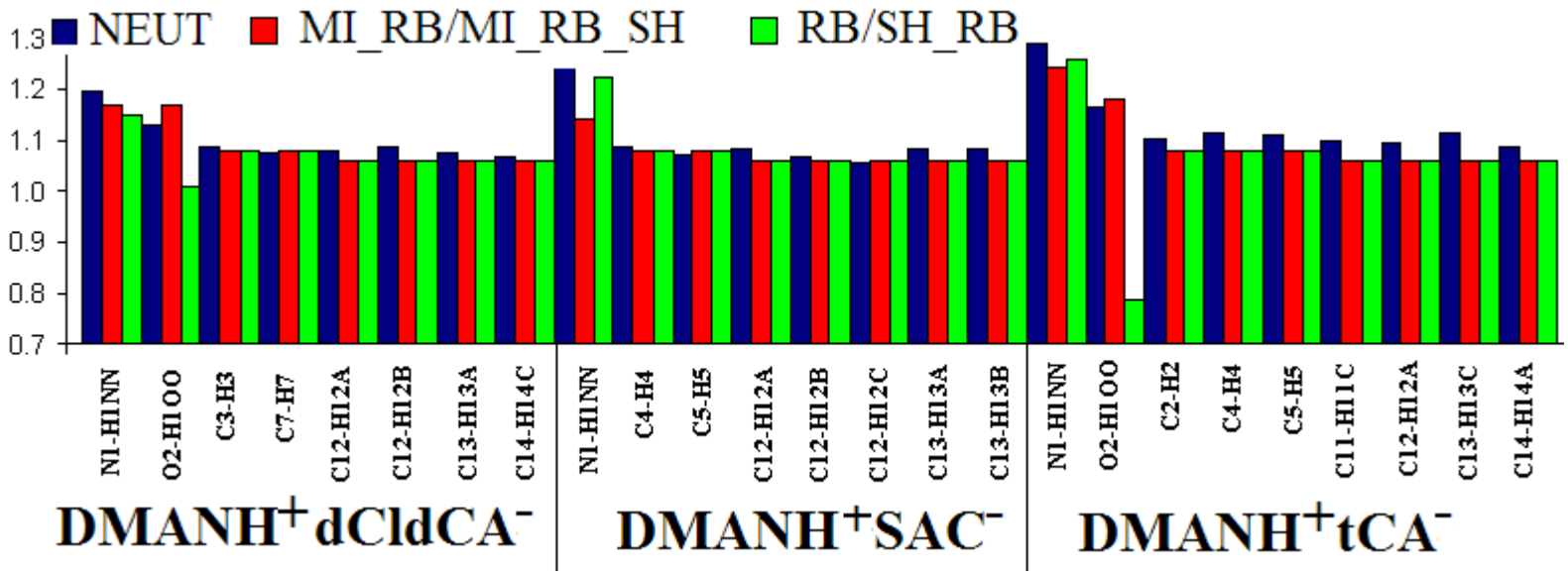
Different treatments of hydrogen atoms in experimental charge density studies and their consequences are discussed. Geometry and topological parameters obtained after applying four different models of H-atoms in multipolar refinement on the high resolution X-ray data only were compared with the results obtained for the referential joint high resolution X-ray/neutron refinement. The geometry and topological critical point and integrated parameters the closest to the referential ones were obtained after a mixed refinement (high-order refinement of heavy atoms, low angle refinement of hydrogen atoms and elongation of the X-H distance to the average neutron bond lengths) supplemented by an estimation of anisotropic thermal motion of H-atoms using the SHADE program. Such a procedure works very well even for the strong hydrogen bonds. The worst fit to the reference results for both critical point and integrated parameters was obtained when *only* the standardisation to the average neutron X-H distances was applied. Also the heavy atom parameters are systematically influenced by the hydrogen atom modeling.

In order to compare topological and integrated properties calculated for hydrogen and even non-hydrogen atoms in multipolar refinement when there is no neutron data, the same treatment of hydrogen atoms (ideally the mixed refinement + SHADE) should be applied.

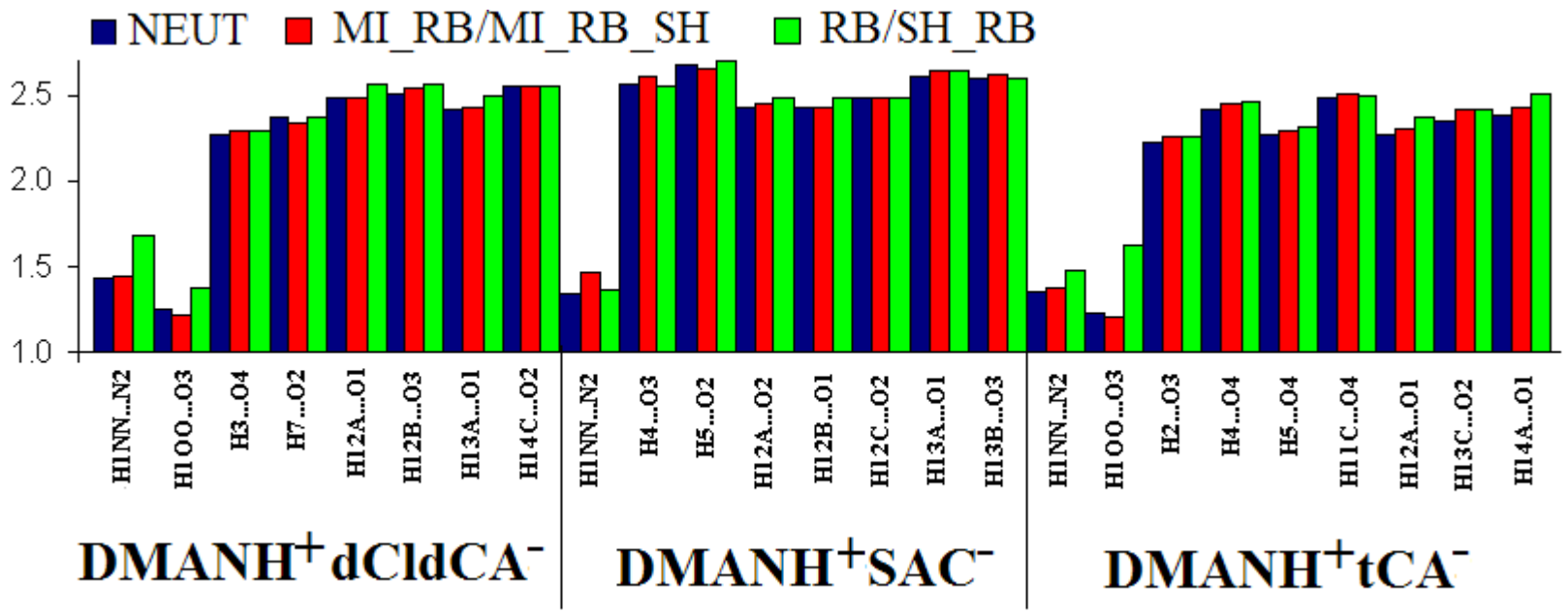
Table S1. Geometry of strong and week hydrogen bonds.

			D-H [Å]	H...A [Å]	D..A [Å]	<DHA[°]
DMANH+tCA-	**N1-H1NN...N2**	NEUT	1.29	1.36	2.600	157.92
		MI_OR/MI_SH	1.24	1.39	2.598	162.50
		RES_B/SH	1.26	1.48	2.600	142.73
	O2-H1OO...O3	NEUT	1.17	1.23	2.397	178.78
		MI_OR/MI_SH	1.18	1.21	2.390	177.54
		RES_B/SH	0.79	1.63	2.398	165.63
	C2-H2...O3	NEUT	1.10	2.23	3.309	166.27
		MI_OR/MI_SH	1.08	2.26	3.313	163.50
		RES_B/SH	1.08	2.26	3.310	164.58
	C4-H4...O4	NEUT	1.12	2.41	3.414	148.94
		MI_OR/MI_SH	1.08	2.45	3.412	148.10
		RES_B/SH	1.08	2.46	3.413	146.85
	C5-H5...O4	NEUT	1.11	2.27	3.303	154.43
		MI_OR/MI_SH	1.08	2.29	3.303	155.00
		RES_B/SH	1.08	2.32	3.304	150.80
	C11-H11C...O4	NEUT	1.10	2.48	3.555	166.88
		MI_OR/MI_SH	1.06	2.51	3.552	166.84
		RES_B/SH	1.06	2.50	3.553	174.36
	C12-H12A...O1	NEUT	1.10	2.27	3.113	131.96
		MI_OR/MI_SH	1.06	2.30	3.114	132.61
		RES_B/SH	1.06	2.37	3.114	125.99
	C13-H13C...O2	NEUT	1.11	2.35	3.417	159.74
		MI_OR/MI_SH	1.06	2.41	3.424	159.20
		RES_B/SH	1.06	2.41	3.418	158.57
	C14-H14A...O1	NEUT	1.09	2.39	3.196	129.83
		MI_OR/MI_SH	1.06	2.43	3.210	129.80
		RES_B/SH	1.06	2.51	3.201	122.26
$DMANH^{+}DClDCA^{-}$	**N1-H1NN...N2**	NEUT	1.20	1.43	2.575	156.34
		MI_OR/MI_SH	1.17	1.45	2.574	159.79
		RES_B/SH	1.15	1.68	2.575	130.48
	O2-H1OO...O3	NEUT	1.13	1.26	2.391	178.07

		MI_OR/MI_SH	1.17	1.22	2.386	176.37
		RES_B/SH	1.01	1.38	2.393	173.60
	C3-H3...O4	NEUT	1.09	2.27	3.222	145.77
		MI_OR/MI_SH	1.08	2.29	3.222	143.91
		RES_B/SH	1.08	2.29	3.222	143.80
	C7-H7...O2	NEUT	1.08	2.37	3.318	146.30
		MI_OR/MI_SH	1.08	2.33	3.316	150.43
		RES_B/SH	1.08	2.38	3.318	144.54
	C12-H12A...O1	NEUT	1.08	2.48	3.234	126.33
		MI_OR/MI_SH	1.06	2.49	3.234	126.73
		RES_B/SH	1.06	2.56	3.234	120.50
	C12-H12B...O3	NEUT	1.09	2.51	3.217	121.76
		MI_OR/MI_SH	1.06	2.54	3.217	121.21
		RES_B/SH	1.06	2.57	3.217	119.20
	C13-H13A...O1	NEUT	1.08	2.42	3.172	126.24
		MI_OR/MI_SH	1.06	2.43	3.172	126.38
		RES_B/SH	1.06	2.50	3.172	120.75
	C14-H14C...O2	NEUT	1.07	2.56	3.602	167.06
		MI_OR/MI_SH	1.06	2.56	3.602	169.28
		RES_B/SH	1.06	2.55	3.602	170.31
DMANH+SAC-	**N1-H1NN...N2**	NEUT	1.26	1.35	2.563	159.38
		MI_OR/MI_SH	1.14	1.47	2.561	158.70
		RES_B/SH	1.22	1.37	2.561	162.93
	C12-H12A...O2	NEUT	1.08	2.43	3.400	147.67
		MI_OR/MI_SH	1.06	2.46	3.398	147.56
		RES_B/SH	1.06	2.49	3.398	143.51
	C12-H12B...O1	NEUT	1.07	2.42	3.348	144.30
		MI_OR/MI_SH	1.06	2.43	3.348	143.91
		RES_B/SH	1.06	2.48	3.348	138.11
	C12-H12C...O2	NEUT	1.06	2.49	3.443	149.57
		MI_OR/MI_SH	1.06	2.48	3.443	151.13
		RES_B/SH	1.06	2.49	3.443	149.25
	C13-H13A...O1	NEUT	1.08	2.61	3.501	138.98
		MI_OR/MI_SH	1.06	2.65	3.501	137.37
		RES_B/SH	1.06	2.64	3.501	138.15
	C13-H13B...O3	NEUT	1.08	2.59	3.511	142.12
		MI_OR/MI_SH	1.06	2.63	3.510	140.67
		RES_B/SH	1.06	2.59	3.510	144.71

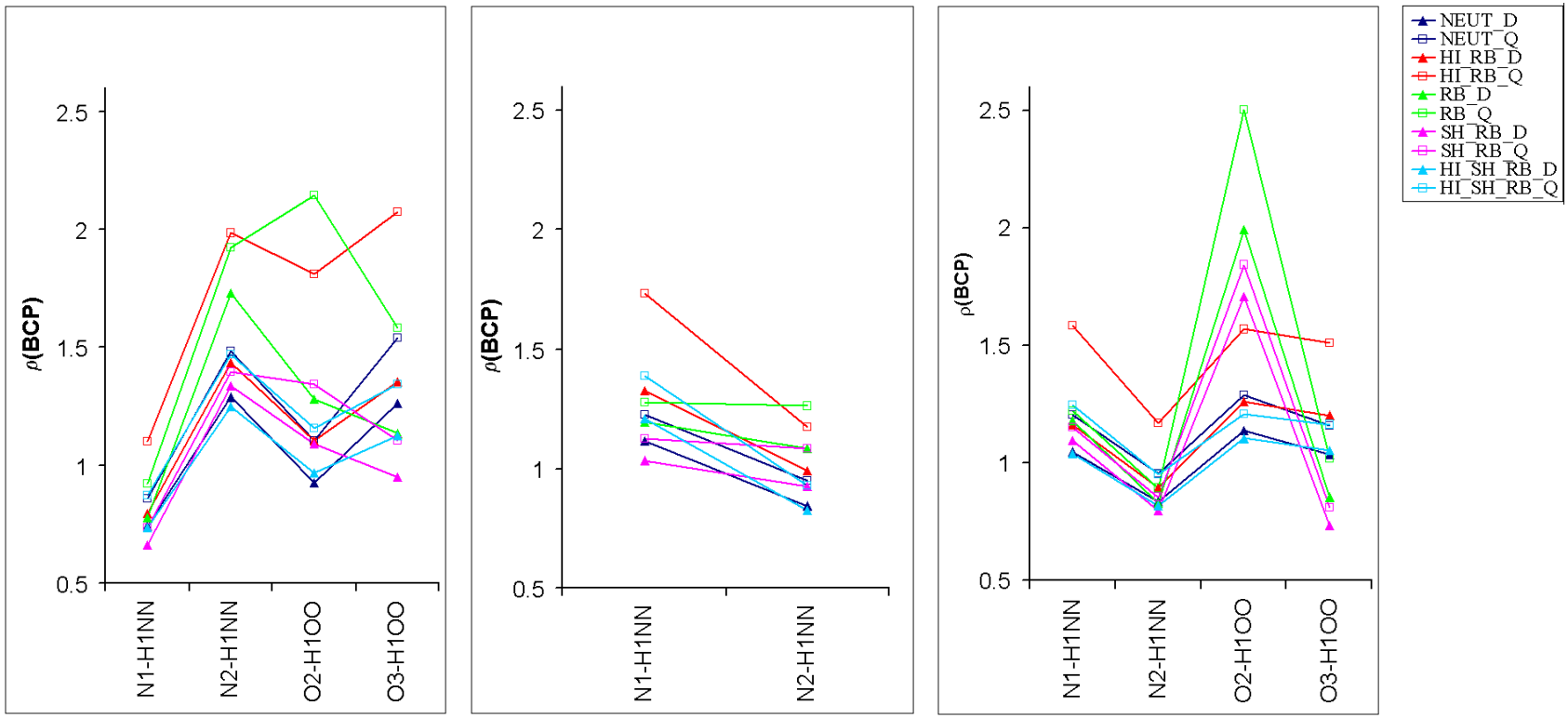

NEUT
MI_RB/MI_RB_SH
RB/SH_RB
1.3
1.2
1.1
1.0
0.9
0.8
0.7
N1-H1NN
O2-H1OO
C3-H3
C7-H7
C12-H12A
C12-H12B
C13-H13A
C14-H14C
N1-H1NN
C4-H4
C5-H5
C12-H12A
C12-H12B
C12-H12C
C13-H13A
C13-H13B
N1-H1NN
O2-H1OO
C2-H2
C4-H4
C5-H5
C11-H11C
C12-H12A
C13-H13C
C14-H14A
DMANH+dCldCA-
DMANH+SAC-
DMANH+tCA-

(a)

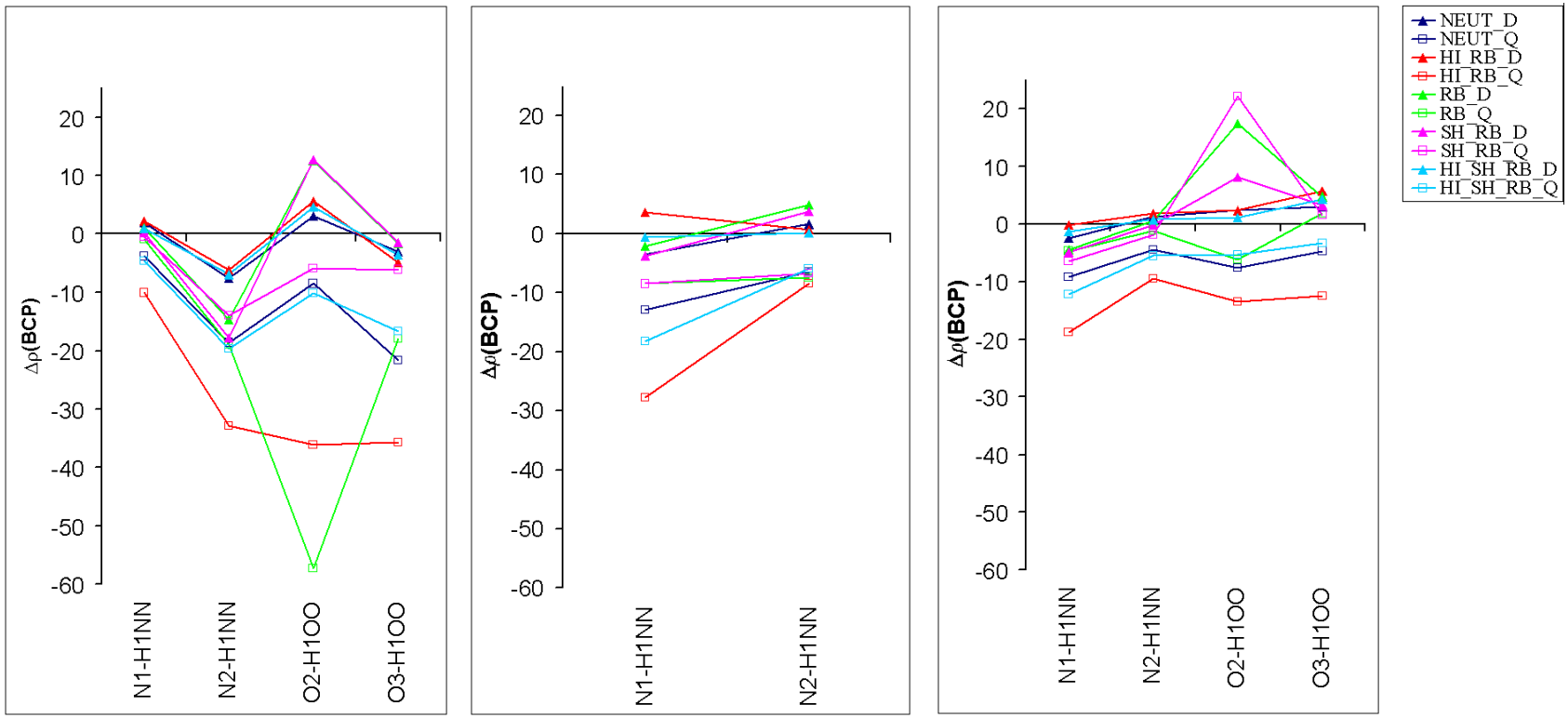


(b)

Fig. S1. Illustration of hydrogen bond structural parameters: (a) D-H bond lengths, (b) H...A distances. Only three most representative cases of refinement are shown for each parameter.

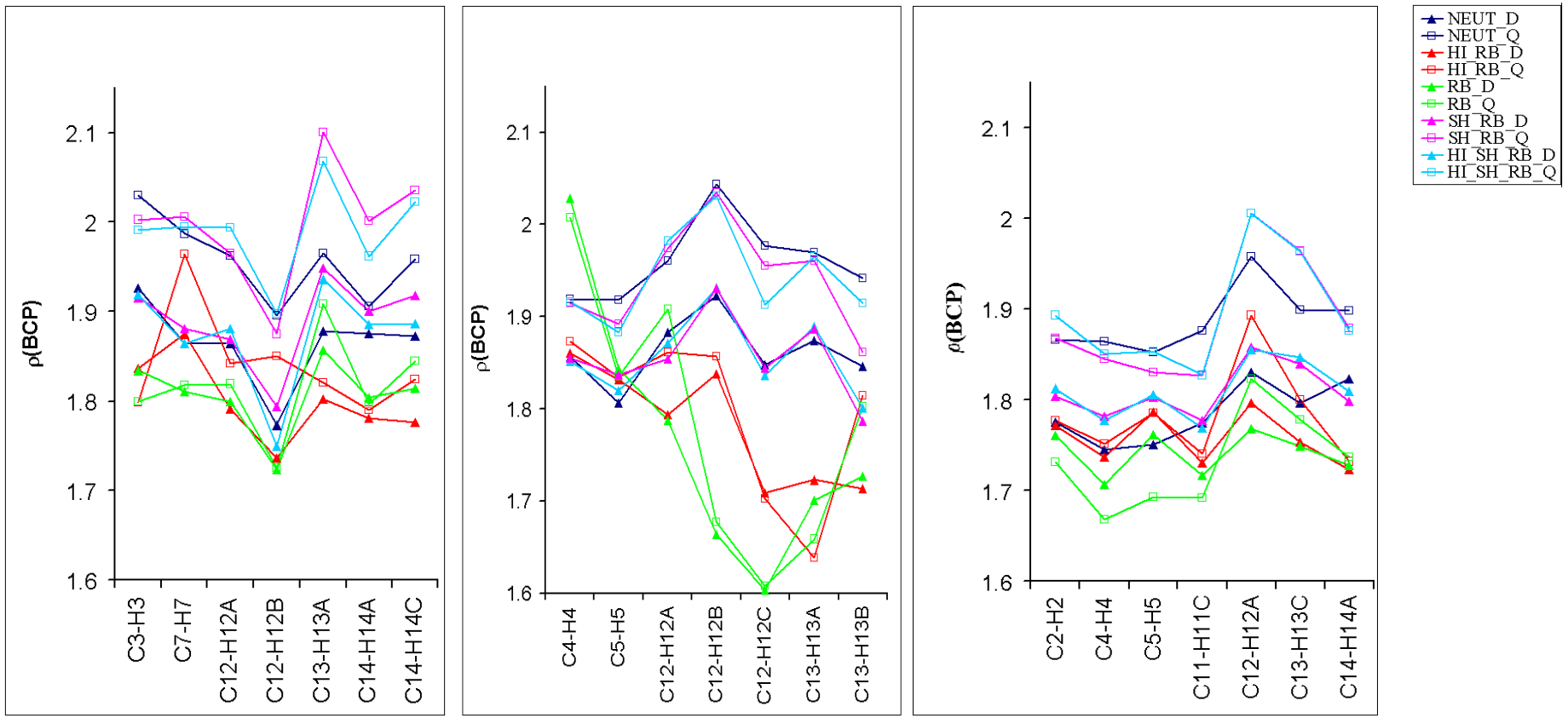

ρ(BCP)
2.5
2
1.5
1
0.5
N1-H1NN
N2-H1NN
O2-H1OO
O3-H1OO
NEUT_D
NEUT_Q
HI_RB_D
HI_RB_Q
RB_D
RB_Q
SH_RB_D
SH_RB_Q
HI_SH_RB_D
HI_SH_RB_Q

(a)

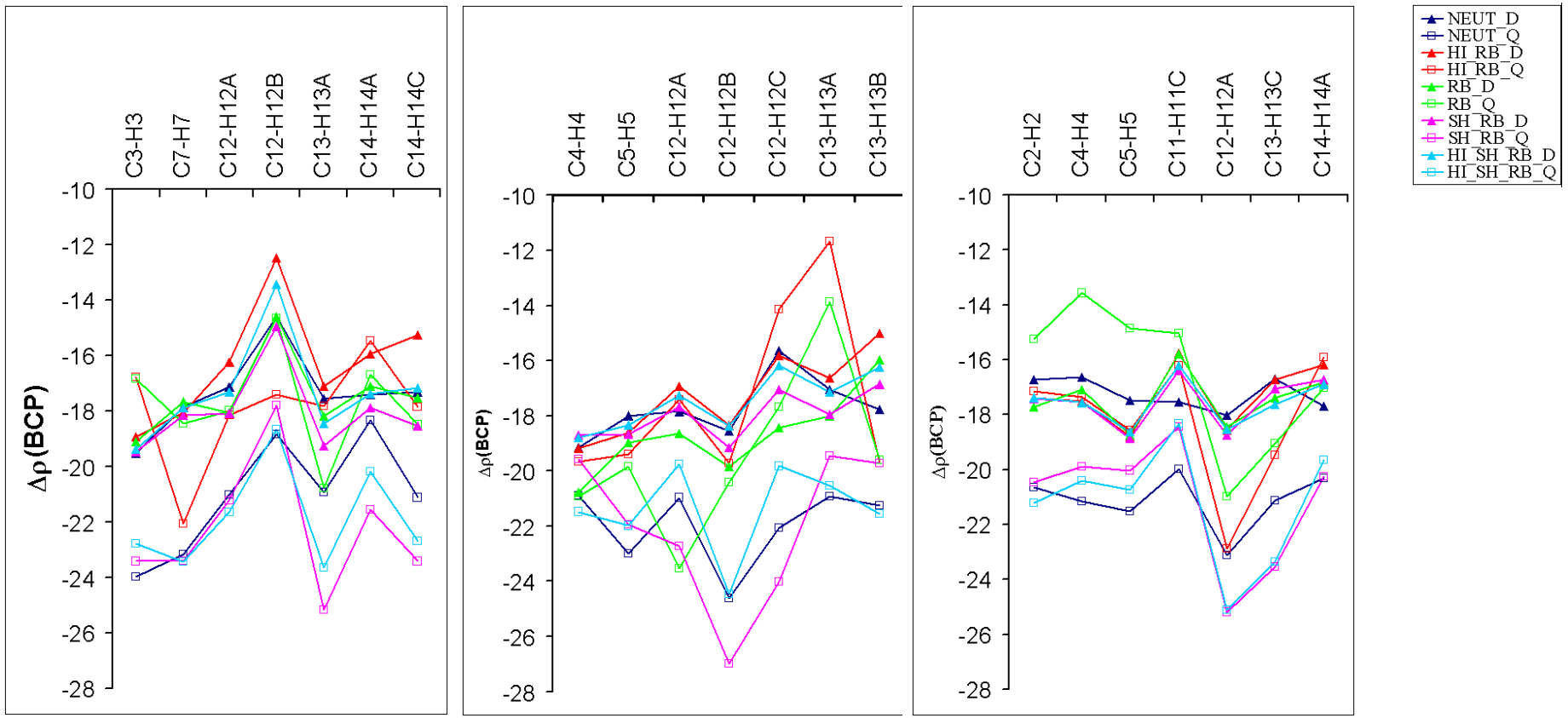


(b)

Fig. S2. (a) Electron density [eÅ^{-3}] and (b) laplacian [eÅ^{-5}] at BCPs for strong hydrogen bonds (N-H...N) and (O-H...O) in DMANH+dCldCA- (left), DMANH+SAC- (middle), DMANH+tCA- (right) calculated applying different hydrogen atom treatments.

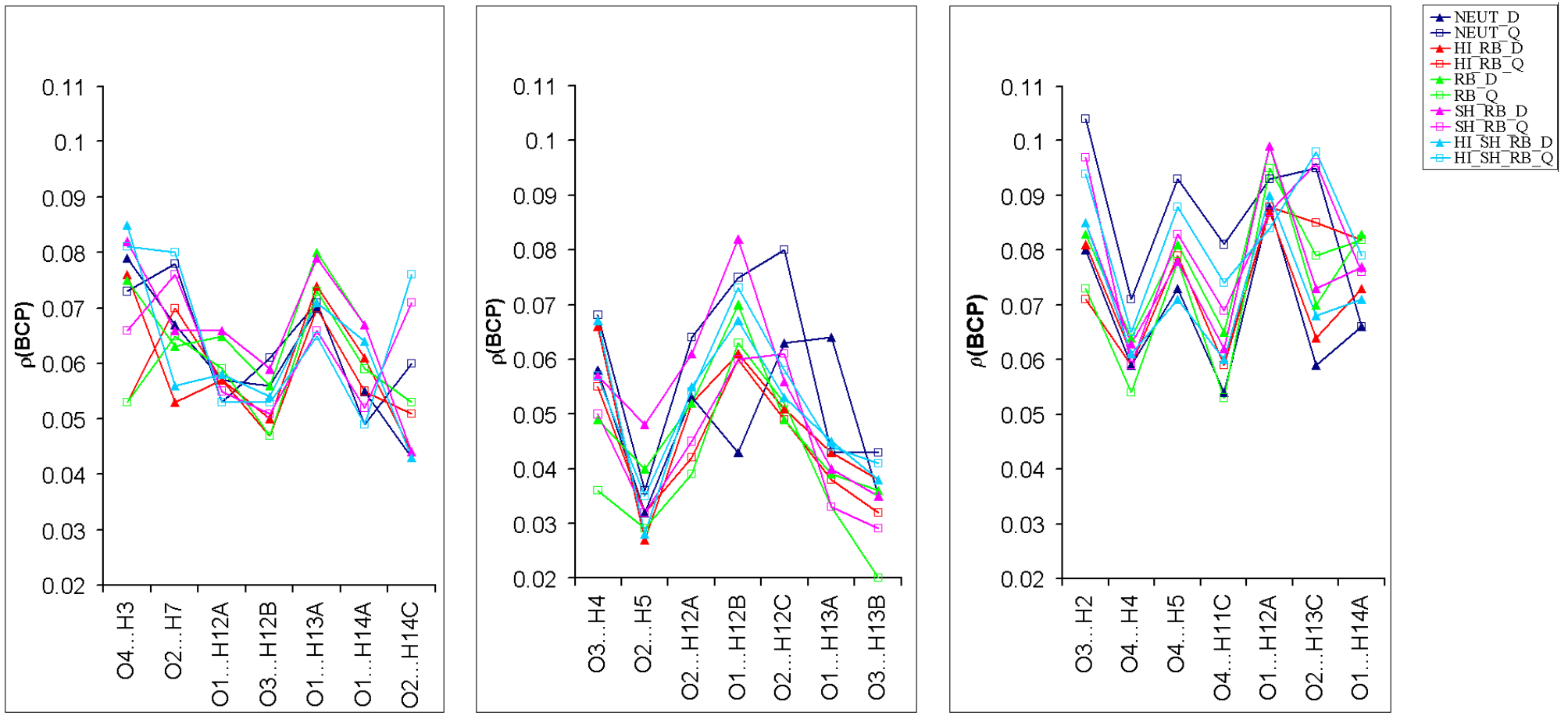

ρ(BCP)
2.1
2
1.9
1.8
1.7
1.6
C3-H3
C7-H7
C12-H12A
C12-H12B
C13-H13A
C14-H14A
C14-H14C
C4-H4
C5-H5
C12-H12A
C12-H12B
C12-H12C
C13-H13A
C13-H13B
C2-H2
C4-H4
C5-H5
C11-H11C
C12-H12A
C13-H13C
C14-H14A
NEUT_D
NEUT_Q
HI_RB_D
HI_RB_Q
RB_D
RB_Q
SH_RB_D
SH_RB_Q
HI_SH_RB_D
HI_SH_RB_Q

(a)

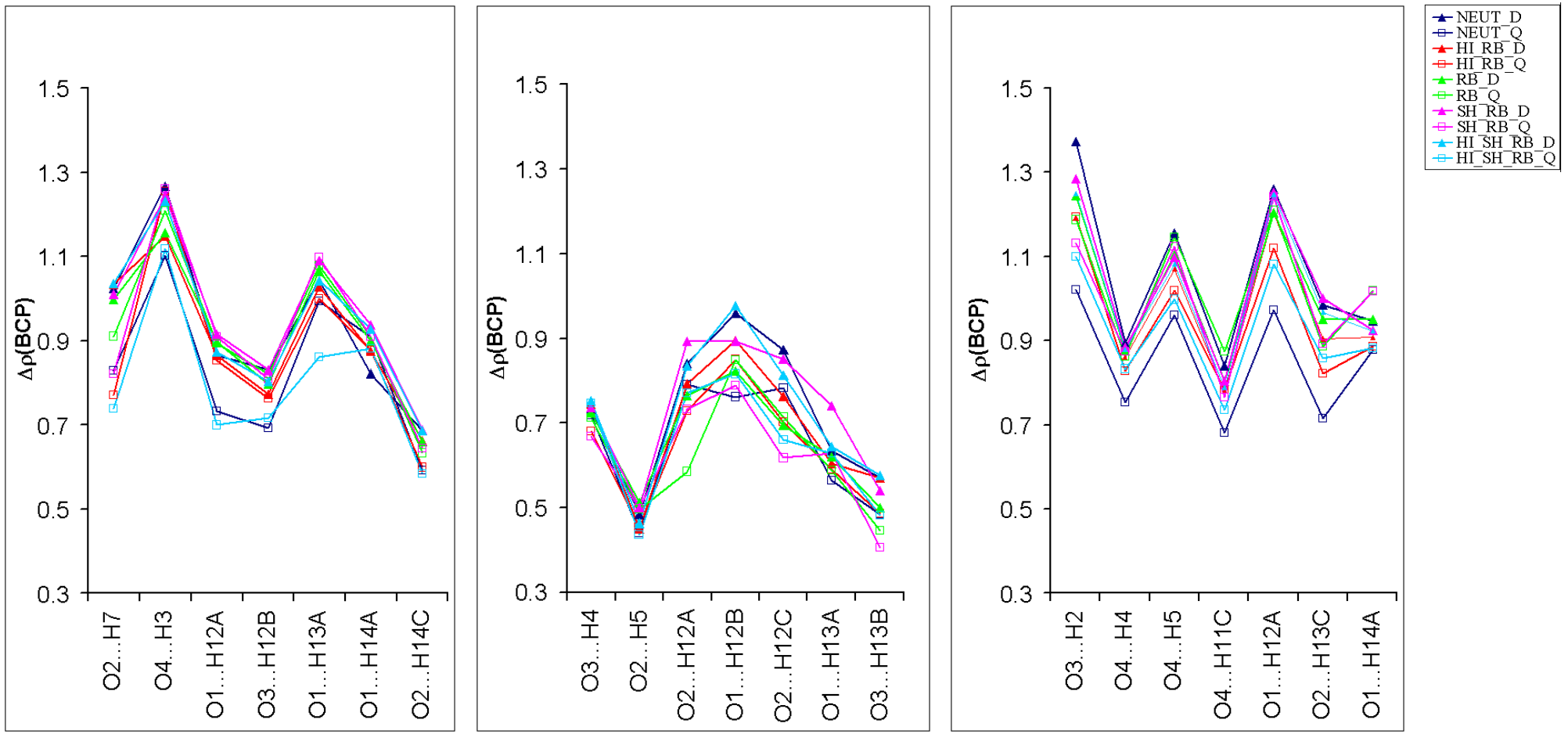


(b)

Fig. S3. (a) Electron density [eÅ^{-3}] and (b) laplacian [eÅ^{-5}] at BCPs for selected covalent C-H bonds in DMANH+dCldCA- (left), DMANH+SAC- (middle), DMANH+tCA- (right) calculated applying different hydrogen atom treatments.

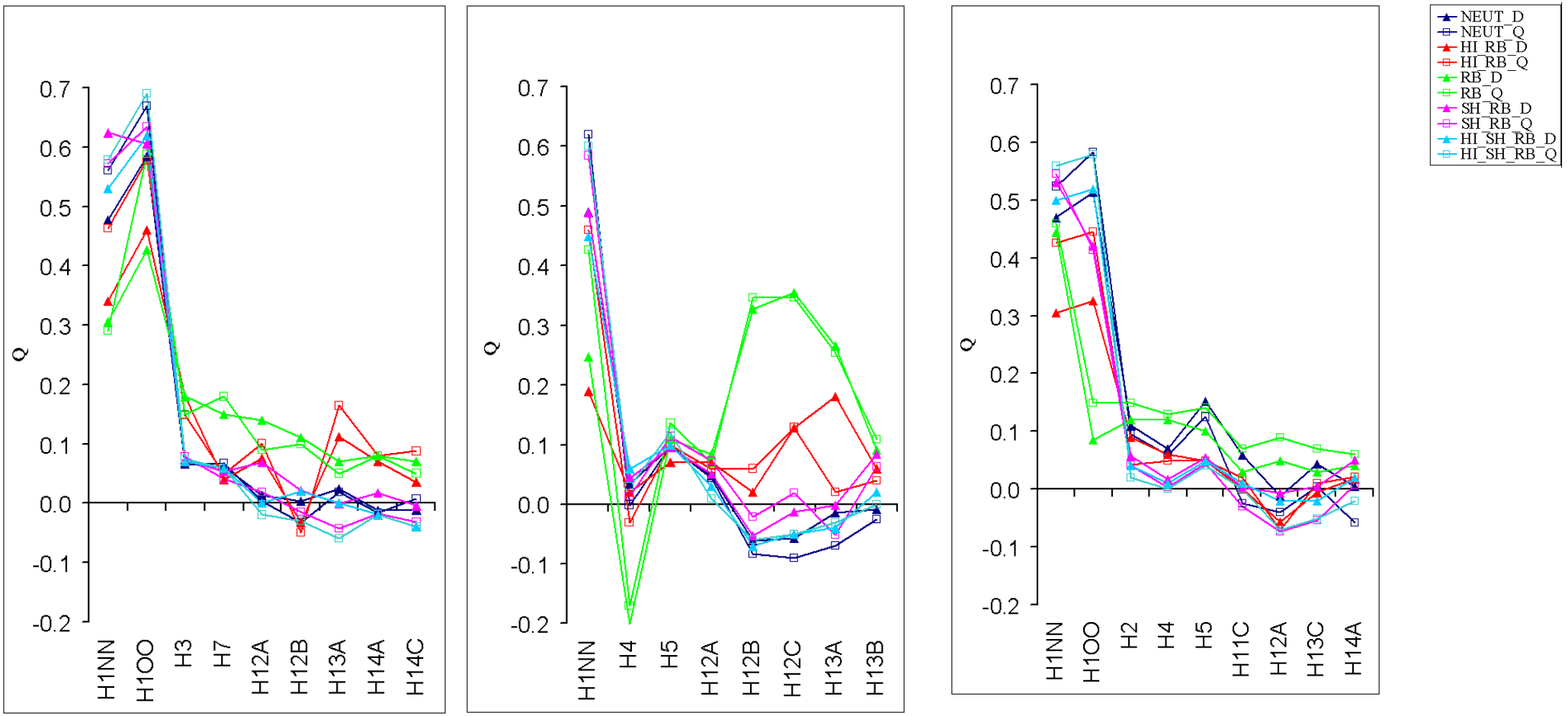

ρ(BCP)
0.11
0.1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
O4...H3
O2...H7
O1...H12A
O3...H12B
O1...H13A
O1...H14A
O2...H14C
O3...H4
O2...H5
O2...H12A
O1...H12B
O2...H12C
O1...H13A
O3...H13B
O3...H2
O4...H4
O4...H5
O4...H11C
O1...H12A
O2...H13C
O1...H14A
NEUT_D
NEUT_Q
HI_RB_D
HI_RB_Q
RB_D
RB_Q
SH_RB_D
SH_RB_Q
HI_SH_RB_D
HI_SH_RB_Q

(a)

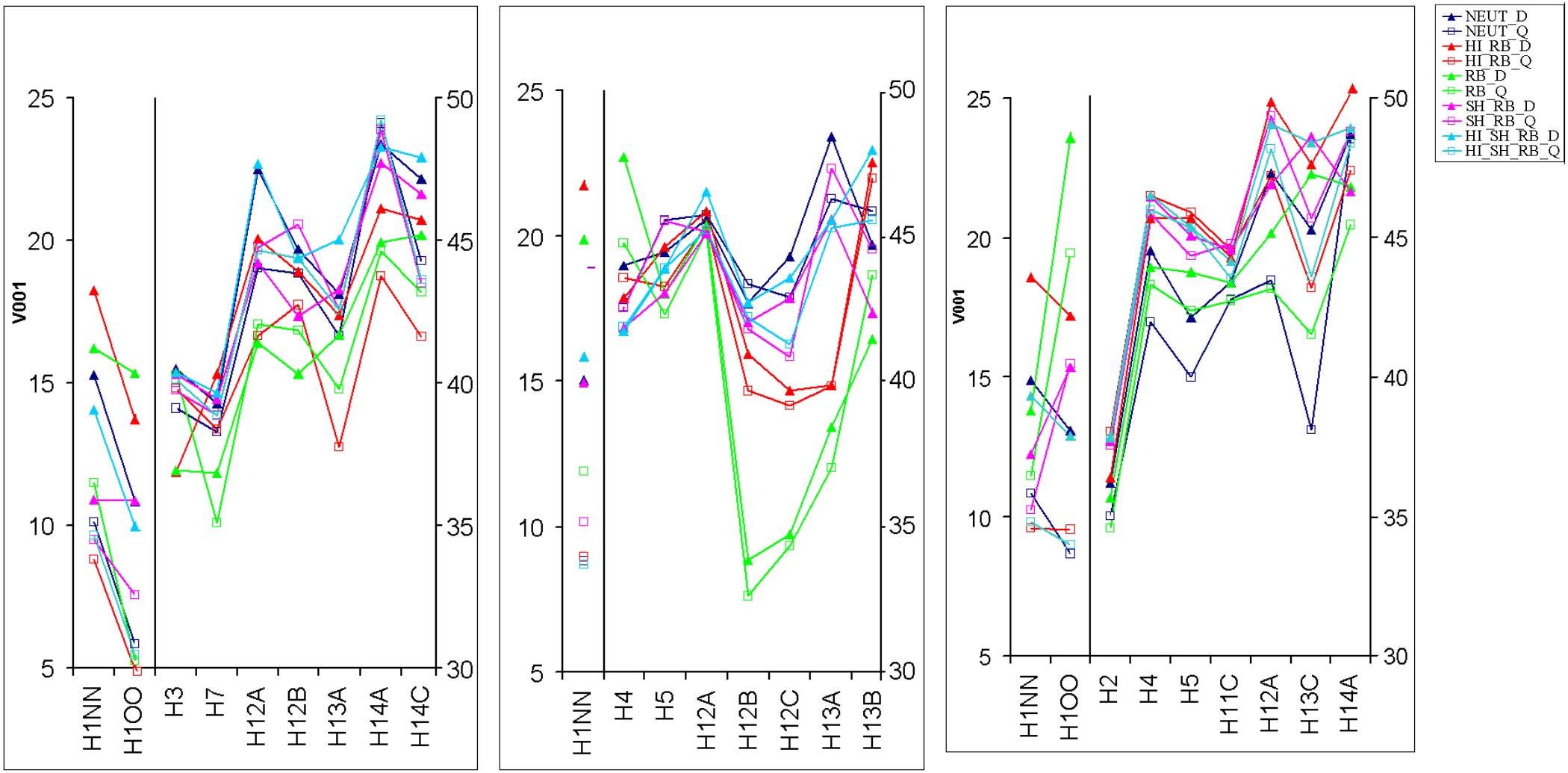


(b)

Fig. S4. (a) Electron density [eÅ^{-3}] and (b) laplacian [eÅ^{-5}] at BCPs for weak C-H...O hydrogen bonds in DMANH+dCldCA- (left), DMANH+SAC- (middle), DMANH+tCA- (right) calculated applying different hydrogen atom treatments.


NEUT_D
NEUT_Q
HI_RB_D
HI_RB_Q
RB_D
RB_Q
SH_RB_D
SH_RB_Q
HI_SH_RB_D
HI_SH_RB_Q
Q
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
-0.2
H1NN
H1OO
H3
H7
H12A
H12B
H13A
H14A
H14C
H1NN
H4
H5
H12A
H12B
H12C
H13A
H13B
H1NN
H1OO
H2
H4
H5
H11C
H12A
H13C
H14A

(a)


V001
25
20
15
10
5
50
45
40
35
30
H1NN
H1OO
H3
H7
H12A
H12B
H13A
H14A
H14C
H4
H5
H12C
H13B
H2
H11C
H13C
NEUT_D
NEUT_Q
HI_RB_D
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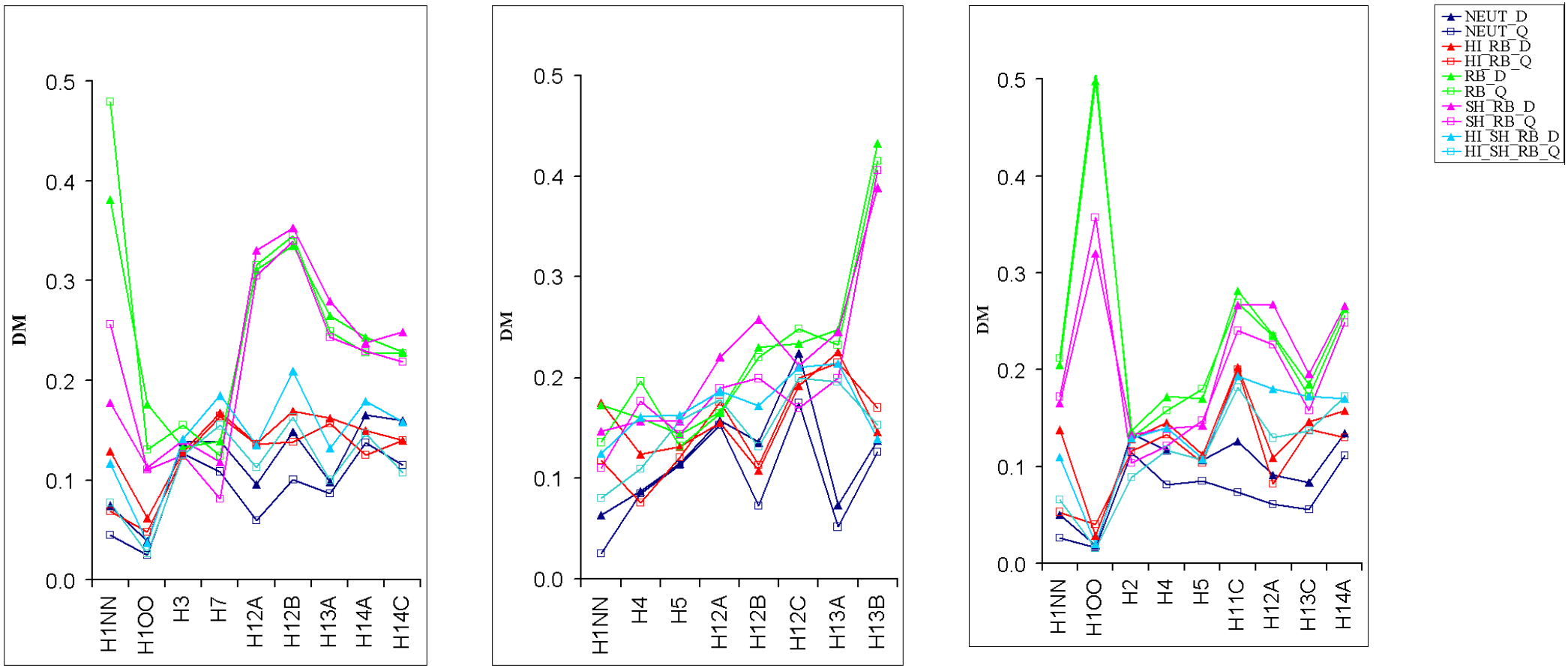
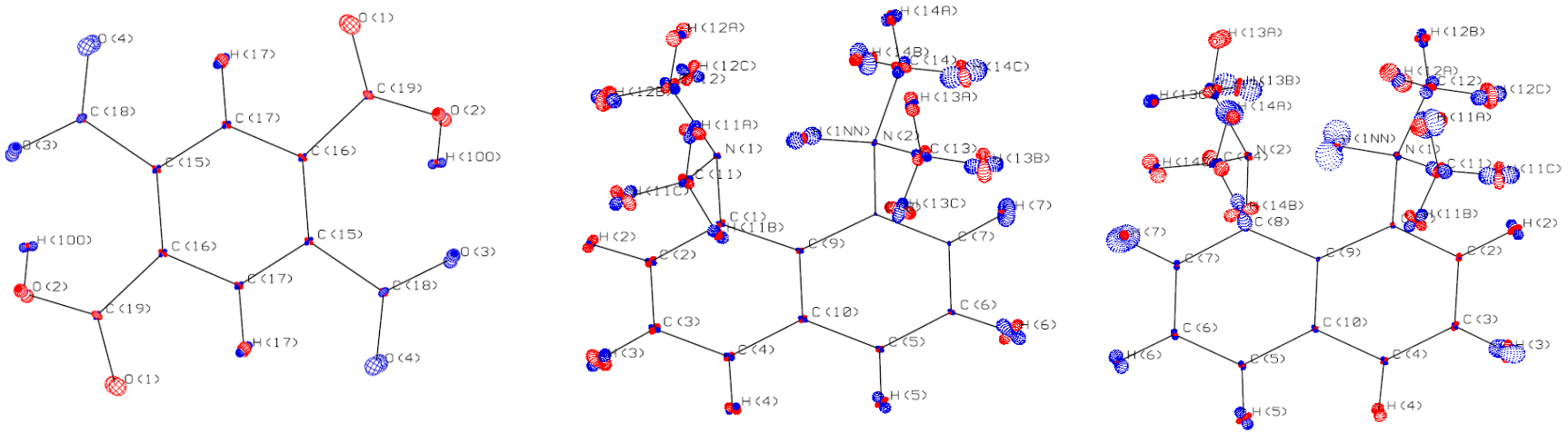
RB_Q
SH_RB_D
SH_RB_Q
HI_SH_RB_D
HI_SH_RB_Q

(b)



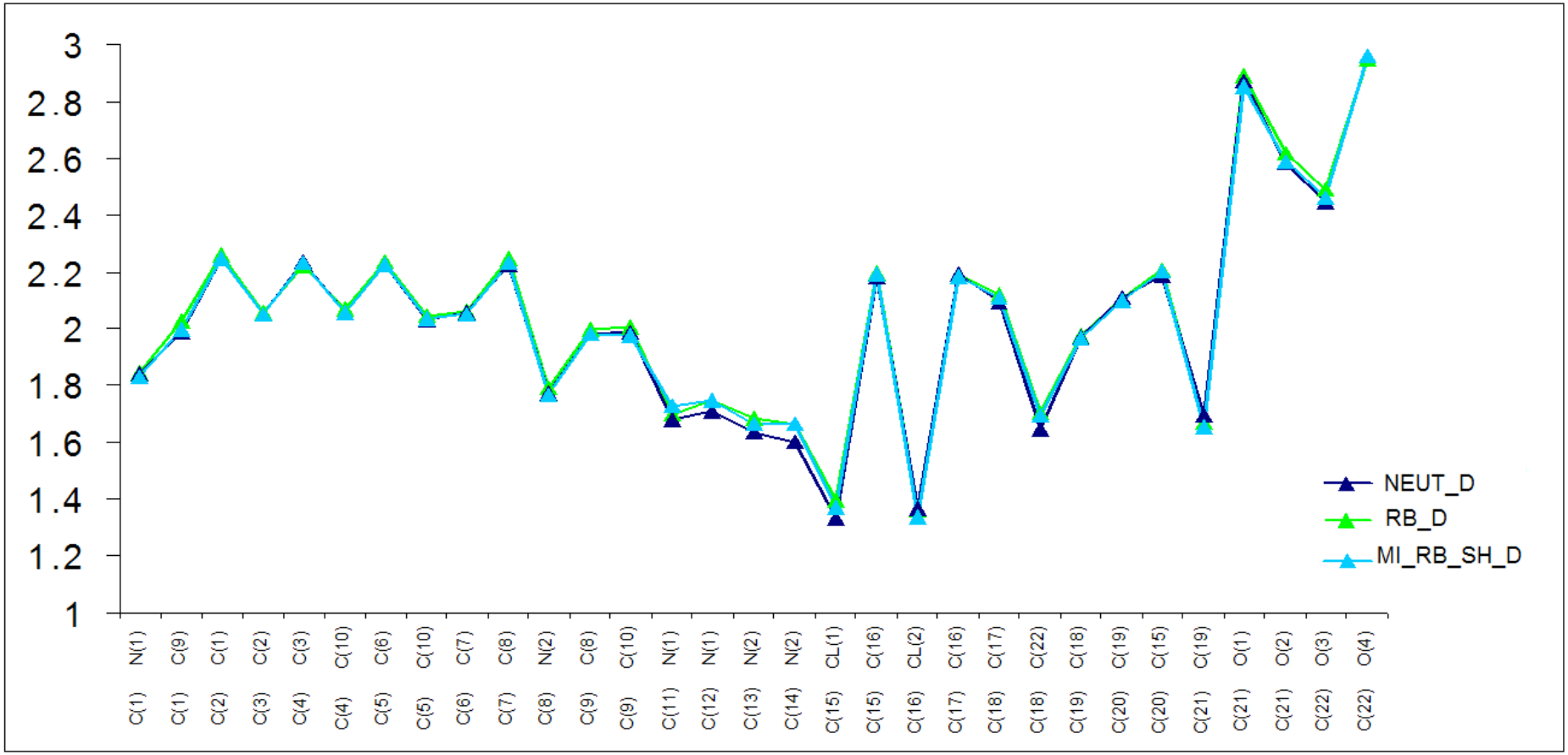
(c)

Fig. S5. (a) Integrated atomic charge [au], (b) integrated atomic volume V001 [au], (c) magnitude of atomic dipole moment [au] for hydrogens involved in hydrogen bonds in DMANH+dCldCA- (left), DMANH+SAC- (middle), DMANH+tCA- (right) calculated applying different hydrogen atom treatments.

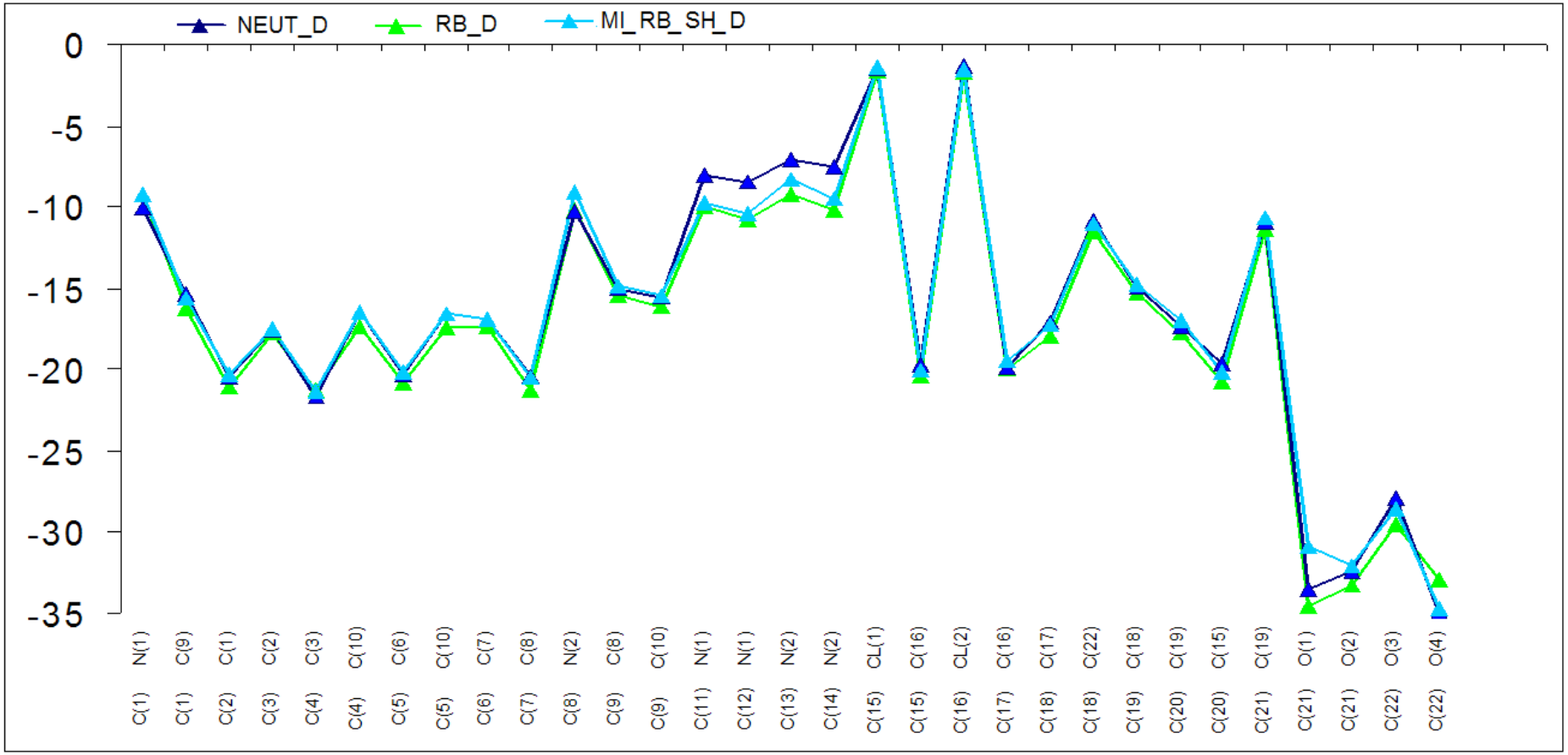


(a) (b) (c)

Fig. S6. PEANUT representation (Hummel, 1990) of the differences in anisotropic ADPs between hydrogen ADPs esitmated by the SHADE program and non-hydrogen ADPs from multipolar refinement, and those from referential neutron data for (a) and (b) DMANH+dCldCA- , (c) DMANH+ from DMANH+SAC-. An overestimation of the ADPs appears in blue. Scale of 1.54 was used for the representation of differences in RMSD surfaces

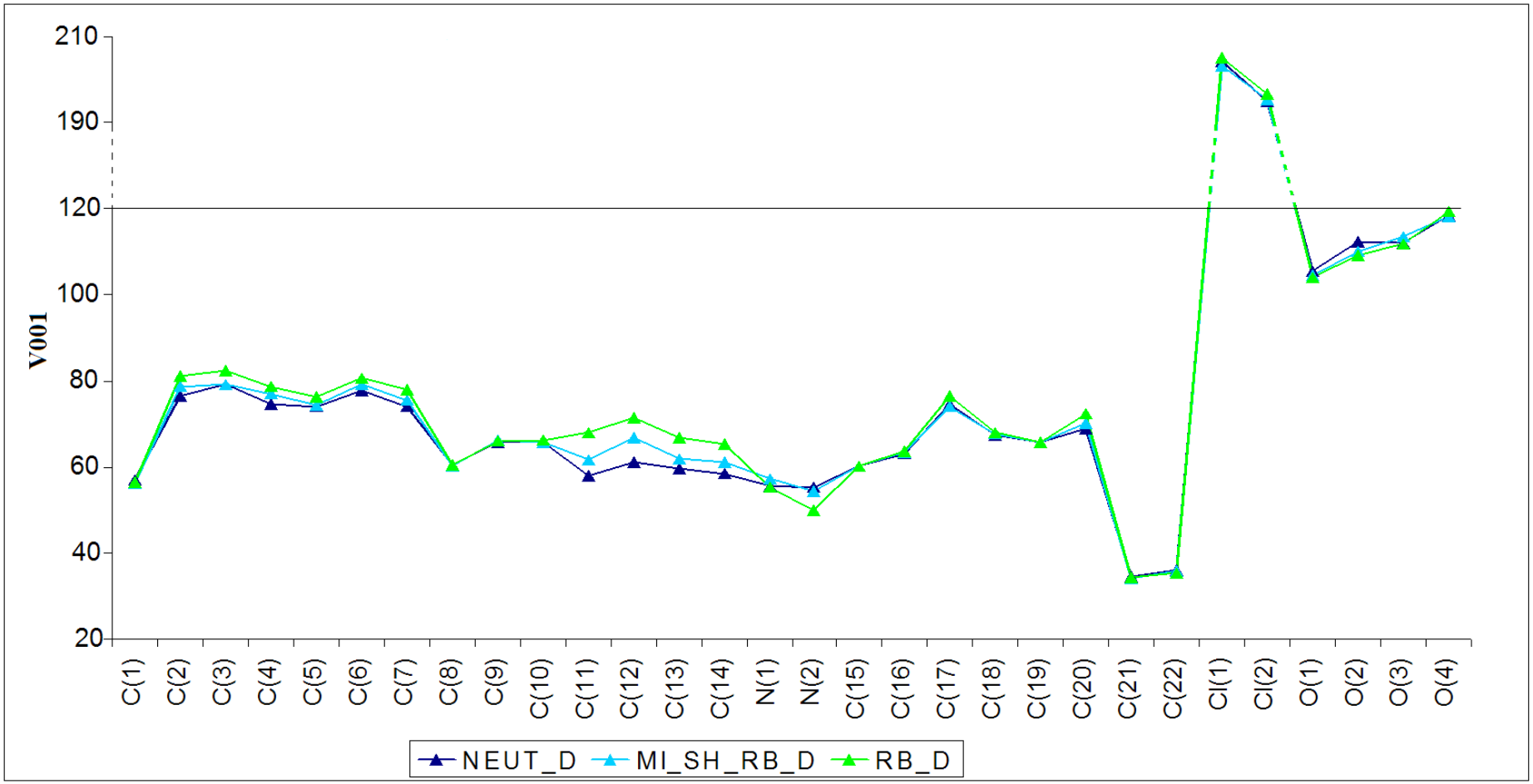

3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
NEUT_D
RB_D
MI_RB_SH_D
N(1) C(1)
C(9) C(1)
C(1) C(2)
C(2) C(3)
C(3) C(4)
C(10) C(4)
C(6) C(5)
C(10) C(5)
C(7) C(6)
C(8) C(7)
N(2) C(8)
C(8) C(9)
C(10) C(9)
N(1) C(11)
N(1) C(12)
N(2) C(13)
N(2) C(14)
CL(1) C(15)
C(16) C(15)
CL(2) C(16)
C(16) C(17)
C(17) C(18)
C(22) C(18)
C(18) C(19)
C(19) C(20)
C(15) C(20)
C(19) C(21)
O(1) C(21)
O(2) C(21)
O(3) C(22)
O(4) C(22)

(a)

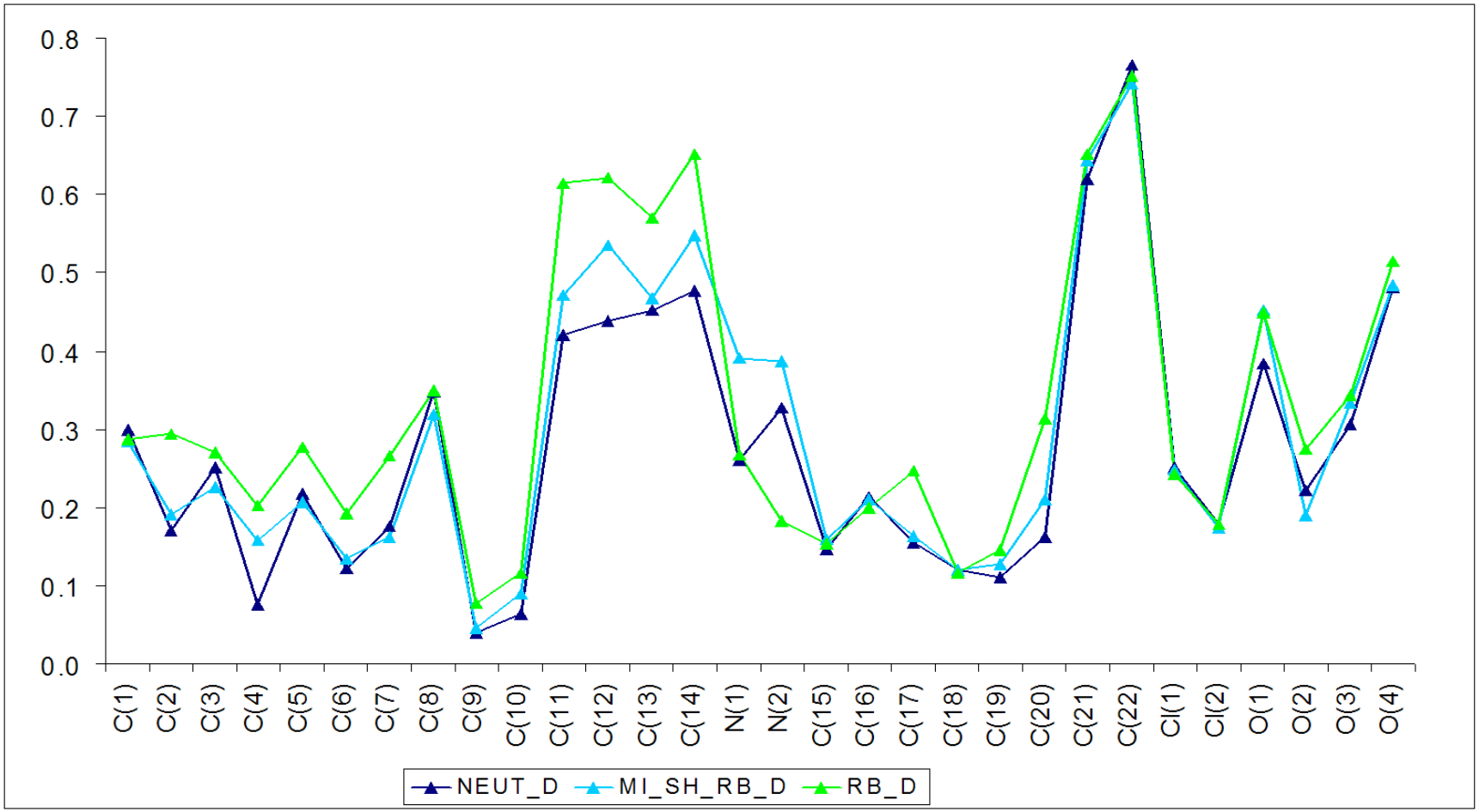


(b)

Fig. S7. (a) Electron density [eÅ^{-3}] and (b) Laplacian [eÅ^{-5}] at BCPs for covalent bonds in DMANH+dCldCA- calculated applying different hydrogen atom treatments.


210
190
120
100
80
60
40
20
V001
C(1)
C(2)
C(3)
C(4)
C(5)
C(6)
C(7)
C(8)
C(9)
C(10)
C(11)
C(12)
C(13)
C(14)
N(1)
N(2)
C(15)
C(16)
C(17)
C(18)
C(19)
C(20)
C(21)
C(22)
Cl(1)
Cl(2)
O(1)
O(2)
O(3)
O(4)
NEUT_D
MI_SH_RB_D
RB_D

(a)



(b)

Fig. S8. (a) Integrated atomic volume [au] and (b) dipole moment magnitude [au] calculated for non-hydrogen atoms for $DMANH^{+}dCldCA^{-}$ by use of three different hydrogen atom models.

DMANH+dCldCA-

	RHO[eÅ^{-3}]									
	NEUT_D	**NEUT_Q**	**MI_RB_D**	**MI_RB_Q**	**RB_D**	**RB_Q**	**SH_RB_D**	**SH_RB_Q**	**MI_SH__RB_D**	**MI_SH__RB_Q**
N1-H1NN	0.743	0.859	0.798	1.102	0.778	0.923	0.663	0.737	0.738	0.874
N2-H1NN	1.290	1.482	1.437	1.984	1.730	1.924	1.339	1.396	1.248	1.471
O2-H1OO	0.928	1.107	1.105	1.810	1.281	2.145	1.092	1.344	0.969	1.160
O3-H1OO	1.264	1.539	1.355	2.074	1.137	1.584	0.952	1.105	1.128	1.345
O4...H3	0.079	0.073	0.076	0.053	0.075	0.053	0.082	0.066	0.085	0.081
O2...H7	0.067	0.078	0.053	0.070	0.063	0.065	0.066	0.076	0.056	0.080
O1...H12A	0.057	0.053	0.057	0.057	0.065	0.059	0.066	0.055	0.058	0.053
O3...H12B	0.056	0.061	0.050	0.047	0.056	0.047	0.059	0.051	0.054	0.053
O1...H13A	0.070	0.071	0.074	0.070	0.080	0.073	0.079	0.066	0.071	0.065
O1...H14A	0.055	0.049	0.061	0.055	0.067	0.059	0.067	0.052	0.064	0.049
O2...H14C	0.043	0.060	0.044	0.051	0.044	0.053	0.044	0.071	0.043	0.076
C3-H3	1.927	2.030	1.837	1.799	1.834	1.800	1.916	2.003	1.919	1.991
C7-H7	1.864	1.987	1.875	1.964	1.811	1.818	1.881	2.006	1.864	1.995
C12-H12A	1.865	1.963	1.791	1.842	1.800	1.819	1.869	1.965	1.881	1.994
C12-H12B	1.773	1.896	1.736	1.851	1.724	1.725	1.794	1.875	1.750	1.898
C13-H13A	1.878	1.965	1.802	1.821	1.857	1.909	1.949	2.101	1.936	2.068
C14-H14A	1.876	1.906	1.781	1.790	1.804	1.797	1.901	2.001	1.886	1.962
C14-H14C	1.873	1.959	1.776	1.825	1.815	1.845	1.918	2.036	1.887	2.022

DMANH+dCldCA
-

LAPL[eÅ^{-5}]

	NEUT_D	NEUT_Q	MI_RB_D	MI_RB_Q	RB_D	RB_Q	SH_RB_D	SH_RB_Q	MI_SH__RB_D	MI_SH__RB_Q
N1-H1NN	1.893	-3.804	2.236	-10.099	1.124	-0.958	0.296	-0.436	1.036	-4.605
N2-H1NN	-7.487	-18.619	-6.198	-32.853	-14.653	-18.924	-17.798	-14.014	-6.973	-19.721
O2-H1OO	2.990	-8.479	5.583	-36.112	12.482	-57.242	12.735	-5.799	4.646	-10.119
O3-H1OO	-3.061	-21.633	-4.878	-35.613	-1.600	-17.959	-1.489	-6.071	-3.590	-16.660
O2...H7	1.024	0.828	1.034	0.770	0.997	0.910	1.010	0.820	1.036	0.738
O4...H3	1.267	1.102	1.148	1.255	1.156	1.208	1.244	1.261	1.232	1.118
O1...H12A	0.864	0.732	0.864	0.852	0.896	0.894	0.915	0.909	0.873	0.700
O3...H12B	0.831	0.693	0.773	0.762	0.797	0.821	0.831	0.809	0.803	0.716
O1...H13A	1.042	0.993	1.027	1.000	1.065	1.078	1.091	1.098	1.043	0.861
O1...H14A	0.821	0.910	0.875	0.878	0.900	0.909	0.937	0.910	0.928	0.881
O2...H14C	0.686	0.592	0.662	0.599	0.661	0.633	0.687	0.644	0.686	0.584
C3-H3	-19.543	-23.977	-18.936	-16.785	-19.100	-16.819	-19.457	-23.426	-19.380	-22.801
C7-H7	-17.864	-23.175	-18.065	-22.049	-17.656	-18.447	-18.149	-23.405	-17.896	-23.460
C12-H12A	-17.117	-21.016	-16.249	-18.140	-18.066	-17.989	-18.098	-21.236	-17.309	-21.662
C12-H12B	-14.612	-18.854	-12.485	-17.411	-14.605	-14.641	-14.950	-17.774	-13.438	-18.662
C13-H13A	-17.547	-20.912	-17.095	-17.810	-18.185	-20.759	-19.258	-25.175	-18.456	-23.641
C14-H14A	-17.402	-18.341	-15.929	-15.460	-17.094	-16.707	-17.897	-21.566	-17.370	-20.191
C14-H14C	-17.318	-21.119	-15.264	-17.868	-17.535	-18.504	-18.542	-23.430	-17.153	-22.699

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	NEUT_D	NEUT_Q	MI_RB_D	MI_RB_Q	RB_D	RB_Q	SH_RB_D	SH_RB_Q	MI_SH__RB_D	MI_SH__RB_Q
N1-H1NN	1.115	1.226	1.328	1.732	1.196	1.277	1.035	1.124	1.209	1.389
N2-H1NN	0.844	0.950	0.990	1.174	1.084	1.261	0.927	1.084	0.828	0.929
O3...H4	0.058	0.068	0.066	0.055	0.049	0.036	0.057	0.050	0.067	0.057
O2...H5	0.032	0.036	0.027	0.032	0.040	0.029	0.048	0.032	0.028	0.035
O2...H12A	0.053	0.064	0.052	0.042	0.052	0.039	0.061	0.045	0.055	0.054
O1...H12B	0.043	0.075	0.061	0.060	0.070	0.063	0.082	0.060	0.067	0.073
O2...H12C	0.063	0.080	0.051	0.049	0.049	0.052	0.056	0.061	0.053	0.058
O1...H13A	0.064	0.043	0.043	0.038	0.039	0.033	0.040	0.033	0.045	0.044
O3...H13B	0.035	0.043	0.038	0.032	0.036	0.020	0.035	0.029	0.038	0.041
C4-H4	1.856	1.919	1.860	1.873	2.028	2.007	1.855	1.914	1.851	1.916
C5-H5	1.806	1.918	1.832	1.834	1.843	1.835	1.837	1.892	1.820	1.883
C12-H12A	1.883	1.961	1.794	1.861	1.787	1.908	1.854	1.974	1.871	1.982
C12-H12B	1.923	2.043	1.838	1.857	1.664	1.677	1.930	2.034	1.931	2.031
C12-H12C	1.848	1.977	1.709	1.702	1.603	1.608	1.844	1.955	1.836	1.913
C13-H13A	1.874	1.969	1.723	1.638	1.701	1.659	1.887	1.961	1.889	1.965
C13-H13B	1.846	1.942	1.714	1.814	1.727	1.802	1.786	1.861	1.801	1.914

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	NEUT_D	NEUT_Q	MI_RB_D	MI_RB_Q	RB_D	RB_Q	SH_RB_D	SH_RB_Q	MI_SH__RB_D	MI_SH__RB_Q
N1-H1NN	-3.454	-12.837	3.661	-27.779	-2.083	-8.507	-3.745	-8.537	-0.475	-18.259
N2-H1NN	1.641	-6.489	0.700	-8.416	4.880	-7.400	3.713	-6.725	0.215	-5.807
O3...H4	0.732	0.719	0.744	0.681	0.725	0.713	0.736	0.668	0.753	0.746
O2...H5	0.484	0.440	0.449	0.454	0.512	0.496	0.500	0.499	0.463	0.436
O2...H12A	0.842	0.790	0.793	0.729	0.765	0.585	0.893	0.733	0.835	0.771
O1...H12B	0.960	0.762	0.895	0.850	0.822	0.849	0.894	0.789	0.977	0.816
O2...H12C	0.874	0.782	0.763	0.703	0.693	0.714	0.852	0.617	0.813	0.660
O1...H13A	0.634	0.564	0.603	0.591	0.621	0.588	0.741	0.628	0.645	0.628
O3...H13B	0.570	0.484	0.570	0.487	0.500	0.446	0.540	0.406	0.576	0.482
C4-H4	-19.145	-20.879	-19.185	-19.680	-20.761	-20.910	-18.698	-19.572	-18.776	-21.474
C5-H5	-17.985	-22.994	-18.614	-19.386	-18.973	-19.849	-18.693	-21.928	-18.328	-21.990
C12-H12A	-17.844	-20.979	-16.925	-17.425	-18.643	-23.528	-17.680	-22.718	-17.259	-19.749
C12-H12B	-18.565	-24.606	-18.352	-19.723	-19.844	-20.411	-19.137	-26.990	-18.381	-24.478
C12-H12C	-15.643	-22.054	-15.826	-14.139	-18.428	-17.690	-17.061	-24.013	-16.171	-19.815
C13-H13A	-17.060	-20.910	-16.637	-11.673	-18.018	-13.869	-17.958	-19.434	-17.130	-20.539
C13-H13B	-17.779	-21.252	-14.995	-19.736	-15.974	-19.604	-16.855	-19.723	-16.253	-21.560

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	NEUT_D	NEUT_Q	MI_RB_D	MI_RB_Q	RB_D	RB_Q	SH_RB_D	SH_RB_Q	MI_SH__RB_D	MI_SH__RB_Q
N1-H1NN	1.046	1.206	1.159	1.584	1.178	1.223	1.095	1.152	1.038	1.247
N2-H1NN	0.837	0.956	0.895	1.169	0.826	0.893	0.798	0.855	0.818	0.951
O2-H1OO	1.138	1.289	1.262	1.568	1.991	2.503	1.709	1.841	1.103	1.207
O3-H1OO	1.035	1.156	1.201	1.508	0.855	1.017	0.733	0.808	1.054	1.163
O3...H2	0.080	0.104	0.081	0.071	0.083	0.073	0.085	0.097	0.085	0.094
O4...H4	0.059	0.071	0.061	0.059	0.064	0.054	0.063	0.059	0.061	0.065
O4...H5	0.073	0.093	0.071	0.079	0.081	0.078	0.078	0.083	0.071	0.088
O4...H11C	0.054	0.081	0.060	0.059	0.065	0.053	0.062	0.069	0.060	0.074
O1...H12A	0.088	0.093	0.087	0.088	0.099	0.095	0.099	0.087	0.090	0.084
O2...H13C	0.059	0.095	0.064	0.085	0.070	0.079	0.073	0.096	0.068	0.098
O1...H14A	0.066	0.066	0.073	0.082	0.083	0.082	0.077	0.076	0.071	0.079
C2-H2	1.775	1.866	1.771	1.777	1.760	1.731	1.804	1.868	1.812	1.893
C4-H4	1.745	1.864	1.736	1.751	1.706	1.668	1.781	1.845	1.777	1.850
C5-H5	1.750	1.852	1.786	1.785	1.761	1.693	1.803	1.830	1.805	1.853
C11-H11C(A)	1.774	1.876	1.730	1.740	1.716	1.692	1.777	1.826	1.769	1.827
C12-H12A(B)	1.830	1.957	1.796	1.893	1.768	1.823	1.858	2.005	1.855	2.005
C13-H13C(B)	1.796	1.899	1.753	1.800	1.749	1.778	1.839	1.964	1.846	1.963
C14-H14A(B)	1.823	1.898	1.723	1.732	1.728	1.736	1.798	1.879	1.809	1.876

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	NEUT_D	NEUT_Q	MI_RB_D	MI_RB_Q	RB_D	RB_Q	SH_RB_D	SH_RB_Q	MI_SH__RB_D	MI_SH__RB_Q
N1-H1NN	-2.522	-9.197	-0.141	-18.708	-4.427	-4.724	-4.882	-6.460	-1.254	-12.133

N2-H1NN	1.300	-4.374	1.861	-9.526	0.509	-1.198	-0.233	-1.856	0.725	-5.565
O2-H1OO	2.313	-7.537	2.323	-13.491	17.465	-6.142	8.131	22.189	1.165	-5.328
O3-H1OO	2.963	-4.706	5.730	-12.462	4.804	1.835	3.376	1.690	4.313	-3.277
O3...H2	1.373	1.022	1.194	1.194	1.245	1.187	1.283	1.131	1.250	1.100
O4...H4	0.894	0.752	0.860	0.827	0.875	0.861	0.884	0.874	0.879	0.833
O4...H5	1.156	0.961	1.069	1.018	1.104	1.146	1.097	1.123	1.081	0.998
O4...H11C	0.839	0.681	0.780	0.783	0.804	0.873	0.804	0.765	0.789	0.736
O1...H12A	1.260	0.973	1.202	1.118	1.203	1.210	1.252	1.242	1.246	1.081
O2...H13C	0.985	0.715	0.905	0.823	0.951	0.886	1.002	0.892	0.967	0.859
O1...H14A	0.947	0.878	0.907	0.886	0.950	1.019	0.925	1.016	0.923	0.882
C2-H2	-16.737	-20.659	-17.400	-17.148	-17.745	-15.264	-17.426	-20.467	-17.387	-21.234
C4-H4	-16.641	-21.165	-17.506	-17.363	-17.093	-13.573	-17.564	-19.917	-17.556	-20.416
C5-H5	-17.475	-21.519	-18.800	-18.567	-18.765	-14.841	-18.855	-20.038	-18.628	-20.742
C11-H11C(A)	-17.526	-19.989	-15.776	-16.204	-15.808	-15.021	-16.411	-18.457	-16.195	-18.317
C12-H12A(B)	-18.015	-23.133	-18.548	-22.896	-18.456	-20.970	-18.757	-25.183	-18.516	-25.109
C13-H13C(B)	-16.700	-21.122	-16.730	-19.469	-17.415	-19.070	-17.047	-23.546	-17.634	-23.357
C14-H14A(B)	-17.683	-20.310	-16.171	-15.933	-16.807	-17.029	-16.739	-20.253	-16.894	-19.653

Q[au] **DMANH+tCA-**

	H1NN	**H1OO**	**H2**	**H4**	**H5**	**H11C**	**H12A**	**H13C**	**H14A**
NEUT_D	0.47	0.51	0.11	0.07	0.15	0.06	-0.01	0.04	0.00

NEUT_Q	0.52	0.58	0.09	0.06	0.12	-0.02	-0.040	0.01	-0.06
MI_RB_D	0.31	0.33	0.09	0.06	0.05	0.00	-0.06	-0.01	0.02
MI_RB_Q	0.43	0.45	0.04	0.05	0.05	0.02	-0.07	0.01	0.02
RB_D	0.44	0.08	0.12	0.12	0.10	0.03	0.05	0.03	0.04
RB_Q	0.46	0.15	0.15	0.13	0.14	0.07	0.09	0.07	0.06
SH_RB_D	0.53	0.42	0.06	0.02	0.05	0.00	-0.01	0.00	0.05
SH_RB_Q	0.55	0.41	0.04	0.00	0.04	-0.03	-0.07	-0.05	0.01
MI_SH_RB_D	0.50	0.52	0.04	0.01	0.05	0.01	-0.02	-0.02	0.02
MI_SH_RB_Q	0.56	0.58	0.02	0.00	0.04	0.00	-0.07	-0.05	-0.02

Q[au] **DMANH+DCLDCA-**

	H1NN	**H1OO**	**H3**	**H7**	**H12A**	**H12B**	**H13A**	**H14A**	**H14C**
NEUT_D	0.48	0.58	0.07	0.06	0.01	0.00	0.02	-0.01	-0.01
NEUT_Q	0.56	0.67	0.07	0.07	0.00	-0.03	0.02	-0.02	0.01
MI_RB_D	0.34	0.46	0.18	0.04	0.08	-0.03	0.11	0.07	0.04
MI_RB_Q	0.46	0.58	0.15	0.05	0.10	-0.05	0.17	0.08	0.09
RB_D	0.31	0.43	0.18	0.15	0.14	0.11	0.07	0.08	0.07
RB_Q	0.29	0.59	0.15	0.18	0.09	0.10	0.05	0.08	0.05
SH_RB_D	0.62	0.61	0.07	0.05	0.07	0.02	0.00	0.02	0.00
SH_RB_Q	0.57	0.64	0.08	0.04	0.02	-0.02	-0.04	-0.02	-0.03
MI_SH_RB_D	0.53	0.62	0.07	0.06	0.00	0.02	0.00	-0.02	-0.04
MI_SH_RB_Q	0.58	0.69	0.08	0.06	-0.02	-0.03	-0.06	-0.02	-0.04

Q[au] **DMANH+SAC-**

	H1NN	**H4**	**H5**	**H12A**	**H12B**	**H12C**	**H13A**	**H13B**
NEUT_D	0.49	0.03	0.10	0.05	-0.06	-0.06	-0.01	-0.01
NEUT_Q	0.62	0.00	0.10	0.04	-0.08	-0.09	-0.07	-0.03
MI_RB_D	0.19	0.02	0.07	0.07	0.02	0.13	0.18	0.06

MI_RB_Q	0.46	-0.03	0.10	0.06	0.06	0.13	0.02	0.04
RB_D	0.25	-0.20	0.11	0.08	0.33	0.36	0.27	0.09
RB_Q	0.43	-0.17	0.14	0.07	0.35	0.35	0.25	0.11
SH_RB_D	0.49	0.04	0.09	0.05	-0.05	-0.01	0.00	0.08
SH_RB_Q	0.58	0.01	0.11	0.07	-0.02	0.02	-0.05	0.06
MI_SH_RB_D	0.45	0.06	0.10	0.03	-0.07	-0.05	-0.04	0.02
MI_SH_RB_Q	0.60	0.03	0.12	0.01	-0.06	-0.05	-0.03	0.00

V001 [au] **DMANH+dCldCA-**

	H1NN	**H1OO**	**H3**	**H7**	**H12A**	**H12B**	**H13A**	**H14A**	**H14C**
NEUT_D	15.26	10.86	40.51	39.29	47.48	44.67	43.12	48.36	47.14
NEUT_Q	10.11	5.86	39.09	38.29	44.01	43.83	41.64	49.09	44.25
MI_RB_D	18.22	13.70	36.89	40.31	45.06	43.90	42.36	46.10	45.70
MI_RB_Q	8.82	4.92	39.81	38.36	41.63	42.71	37.75	43.72	41.61
RB_D	16.21	15.36	36.93	36.82	41.39	40.32	41.71	44.91	45.19
RB_Q	11.47	5.24	40.27	35.08	42.05	41.82	39.76	44.62	43.19
SH_RB_D	10.89	10.88	40.29	39.43	44.21	42.32	43.28	47.71	46.61
SH_RB_Q	9.50	7.53	39.70	38.87	44.75	45.57	42.58	48.85	43.48
MI_SH_RB_D	14.06	9.95	40.38	39.66	47.69	44.37	45.03	48.27	47.91
MI_SH_RB_Q	9.66	5.45	40.10	38.83	44.65	44.38	42.58	49.21	43.64

V001 [au] **DMANH+tCA-**

	H1NN	**H1OO**	**H2**	**H4**	**H5**	**H11C**	**H12A**	**H13C**	**H14A**
NEUT_D	14.91	13.07	36.20	44.54	42.13	43.40	47.30	45.27	48.68
NEUT_Q	10.84	8.66	35.01	41.98	40.00	42.80	43.48	38.11	48.55

MI_RB_D	18.60	17.19	36.41	45.70	45.71	44.30	49.86	47.64	50.19
MI_RB_Q	9.58	9.53	38.06	46.50	45.91	44.55	47.22	43.19	47.41
RB_D	13.79	23.58	35.67	43.96	43.77	43.37	45.18	47.29	46.84
RB_Q	11.45	19.43	34.58	43.32	42.38	42.74	43.17	41.53	45.46
SH_RB_D	12.22	15.37	37.72	46.47	45.07	44.56	46.92	48.64	46.66
SH_RB_Q	10.26	15.49	37.55	45.85	44.35	44.80	49.38	45.71	48.81
MI_SH_RB_D	14.35	12.88	37.87	46.55	45.37	44.17	49.07	48.41	48.94
MI_SH_RB_Q	9.81	8.97	37.80	46.03	45.36	43.53	48.19	43.62	48.37

V001 [au] **DMANH+SAC-**

	H1NN	**H4**	**H5**	**H12A**	**H12B**	**H12C**	**H13A**	**H13B**
NEUT_D	15.05	43.97	44.43	45.59	42.70	44.28	48.44	44.67
NEUT_Q	8.82	42.56	45.53	45.70	43.33	42.89	46.29	45.85
MI_RB_D	21.74	42.86	44.63	45.83	40.93	39.69	39.86	47.53
MI_RB_Q	8.96	43.55	43.25	45.39	39.65	39.15	39.81	46.98
RB_D	19.85	47.69	43.00	45.38	33.85	34.73	38.42	41.44
RB_Q	11.91	44.76	42.30	45.13	32.61	34.35	37.04	43.65
SH_RB_D	14.96	41.83	43.05	45.09	42.05	42.86	45.59	42.36
SH_RB_Q	10.16	42.52	45.49	45.15	41.78	40.84	47.31	44.53
MI_SH_RB_D	15.86	41.72	43.87	46.51	42.72	43.56	45.53	47.95
MI_SH_RB_Q	8.71	41.87	43.89	45.20	42.21	41.26	45.26	45.53

DM[au] **DMANH+tCA-**

	H1NN	**H1OO**	**H2**	**H4**	**H5**	**H11C**	**H12A**	**H13C**	**H14A**
NEUT_D	0.051	0.019	0.134	0.117	0.107	0.127	0.092	0.084	0.135
NEUT_Q	0.026	0.016	0.115	0.081	0.085	0.073	0.061	0.056	0.111
MI_RB_D	0.138	0.029	0.128	0.145	0.112	0.203	0.109	0.146	0.158
MI_RB_Q	0.053	0.041	0.116	0.133	0.103	0.200	0.082	0.138	0.130
RB_D	0.205	0.498	0.137	0.172	0.170	0.282	0.236	0.185	0.263
RB_Q	0.212	0.509	0.130	0.158	0.180	0.269	0.234	0.172	0.256

SH_RB_D	0.166	0.320	0.133	0.139	0.143	0.267	0.268	0.196	0.266
SH_RB_Q	0.172	0.357	0.104	0.121	0.148	0.240	0.226	0.157	0.249
MI_SH_RB_D	0.110	0.020	0.129	0.140	0.108	0.193	0.180	0.173	0.170
MI_SH_RB_Q	0.066	0.016	0.089	0.117	0.107	0.182	0.130	0.137	0.172

DM[au]	**H1NN**	**H1OO**	**H3**	**H7**	**DMANH+dCldCA-H12A**	**H12B**	**H13A**	**H14A**	**H14C**
NEUT_D	0.074	0.038	0.139	0.139	0.096	0.148	0.098	0.165	0.160
NEUT_Q	0.045	0.025	0.127	0.109	0.059	0.100	0.086	0.137	0.115
MI_RB_D	0.129	0.062	0.128	0.167	0.137	0.169	0.162	0.150	0.140
MI_RB_Q	0.068	0.048	0.124	0.164	0.136	0.138	0.157	0.125	0.140
RB_D	0.382	0.176	0.133	0.139	0.311	0.335	0.265	0.243	0.229
RB_Q	0.480	0.131	0.156	0.124	0.316	0.345	0.249	0.228	0.227
SH_RB_D	0.178	0.113	0.140	0.118	0.331	0.353	0.280	0.238	0.248
SH_RB_Q	0.256	0.111	0.126	0.081	0.305	0.340	0.243	0.230	0.218
MI_SH_RB_D	0.117	0.037	0.141	0.185	0.135	0.209	0.132	0.179	0.158
MI_SH_RB_Q	0.077	0.026	0.125	0.155	0.113	0.163	0.100	0.147	0.107

DM[au]	**H1NN**	**H4**	**H5**	**DMANH+SAC-H12A**	**H12B**	**H12C**	**H13A**	**H13B**
NEUT_D	0.064	0.087	0.114	0.158	0.136	0.224	0.073	0.138
NEUT_Q	0.025	0.085	0.113	0.153	0.072	0.175	0.052	0.126
MI_RB_D	0.175	0.124	0.131	0.155	0.108	0.192	0.226	0.146
MI_RB_Q	0.118	0.076	0.121	0.176	0.113	0.200	0.215	0.170
RB_D	0.172	0.160	0.144	0.166	0.230	0.234	0.248	0.433
RB_Q	0.136	0.197	0.132	0.164	0.220	0.248	0.232	0.415
SH_RB_D	0.147	0.156	0.156	0.221	0.258	0.212	0.246	0.389

SH_RB_Q	0.110	0.177	0.143	0.190	0.199	0.170	0.199	0.406
MI_SH_RB_D	0.125	0.161	0.163	0.187	0.172	0.210	0.214	0.139
MI_SH_RB_Q	0.080	0.109	0.158	0.178	0.131	0.200	0.196	0.153