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Supporting Information



A Linear Scaling QM/MM Method to Study Molecular Crystals Using BRABO/CHARMM: Application to 2-(2-methyl-3-chloroanilino) nicotinic acid

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Table 1S: Cartesian coordinates for formamide oxime obtained using the PC model.

Atom	x-coordinate	y-coordinate	z-coordinate
C_1	2.400740	2.119277	1.144288
N_2	3.525684	2.861496	1.130684
N_3	2.065807	1.160509	0.363697
O_4	3.125487	0.907230	-0.598648
H_5	3.712071	3.536698	1.847293
H_6	4.251535	2.683563	0.463351
H_7	1.674831	2.351924	1.905230
H_8	2.728660	0.312631	-1.248949

Table 2S: Cartesian coordinates for formamide oxime obtained using the PCX model.

Atom	x-coordinate	y-coordinate	z-coordinate
C_1	2.403713	2.226544	1.038451
N_2	3.567583	2.887056	1.037236
N_3	2.052259	1.264419	0.262250
O_4	3.128980	0.923370	-0.649753
H_5	3.799242	3.563353	1.747538
H_6	4.340390	2.577331	0.465204
H_7	1.654650	2.529171	1.750912
H_8	2.745648	0.247263	-1.238727

Table 3S: Cartesian coordinates for formamide oxime obtained using the SM model.

Atom	x-coordinate	y-coordinate	z-coordinate
C_1	2.424481	2.097581	1.230013
N_2	3.508782	2.862744	1.145892
N_3	2.100141	1.142900	0.429104
O_4	3.096103	1.000742	-0.606207
H_5	3.740085	3.515868	1.873527
H_6	4.210089	2.673767	0.448551
H_7	1.741973	2.279920	2.040577
H_8	2.764175	0.283949	-1.186501

Table 4S: Cartesian coordinates for formamide oxime obtained using the SMX model.

Atom	x-coordinate	y-coordinate	z-coordinate
C_1	2.418131	2.101413	1.215996
N_2	3.507213	2.861341	1.140564
N_3	2.097494	1.145404	0.415313
O_4	3.103884	0.992245	-0.608175
H_5	3.732340	3.516424	1.868127
H_6	4.216617	2.666816	0.452263
H_7	1.727423	2.290575	2.018276
H_8	2.769590	0.280578	-1.193607

Table 5S: Cartesian coordinates for α-glycine obtained using the PC model.

Atom	x-coordinate	y-coordinate	z-coordinate
O_1	0.863445	1.511882	1.349095
O_2	-1.098302	1.272432	0.265878
N_3	2.017346	0.915706	-1.302942
C_4	0.152685	1.528720	0.307700
C_5	0.835022	1.844458	-1.041230
H_6	2.290944	1.001725	-2.308772
H_7	2.861120	1.161541	-0.726113
H_8	1.732697	-0.057350	-1.063947
H_9	1.206879	2.864662	-1.125053
H_{10}	0.113701	1.690193	-1.834444

Table 6S: Cartesian coordinates for α-glycine obtained using the PCX model.

Atom	x-coordinate	y-coordinate	z-coordinate
O_1	1.215380	1.189538	1.083113
O_2	-0.966478	1.520089	0.698102
N_3	1.726845	1.000134	-1.627684
C_4	0.241231	1.459557	0.329114
C_5	0.518225	1.729409	-1.139172
H_6	1.889247	1.156760	-2.649838
H_7	2.586613	1.289909	-1.114814
H_8	1.611521	-0.014682	-1.471476
H_9	0.677291	2.789333	-1.302300
H_{10}	-0.330815	1.414695	-1.732088

Table 7S: Cartesian coordinates for α-glycine obtained using the SM model.

Atom	x-coordinate	y-coordinate	z-coordinate
O_1	1.304720	1.220804	1.175597
O_2	-0.812982	1.384154	0.482073
N_3	2.191795	1.024401	-1.337163
C_4	0.427136	1.423762	0.288214
C_5	0.911944	1.721646	-1.106606
H_6	2.573786	1.179776	-2.276338
H_7	2.902967	1.299468	-0.645886
H_8	2.080001	0.014627	-1.226495
H_9	1.053211	2.791658	-1.218346
H_{10}	0.185942	1.387980	-1.835396

Table 8S: Cartesian coordinates for α-glycine obtained using the SMX model.

Atom	x-coordinate	y-coordinate	z-coordinate
O_1	1.421793	1.251637	0.930045
O_2	-0.764593	1.571821	0.611107
N_3	1.883233	1.003627	-1.731743
C_4	0.423297	1.482713	0.192829
C_5	0.658221	1.687167	-1.280827
H_6	2.058911	1.159060	-2.738815
H_7	2.718559	1.330096	-1.217261
H_8	1.833300	-0.005460	-1.586180
H_9	0.764429	2.748973	-1.473087
H_{10}	-0.187974	1.320315	-1.845665

Table 9S: Cartesian coordinates for dimethyl 3,6-dichloro-2,5-dihydroxyterephthalate obtained using the PCX model.

Atom	x-coordinate	y-coordinate	z-coordinate
C_1	4.041063	-1.157649	-2.929126
O_2	2.995896	-0.448861	-2.195558
C_3	1.893120	-1.093499	-1.904442
O_4	1.669103	-2.195561	-2.414328
C_5	0.953295	-0.484952	-0.928275
C_6	1.156673	0.692412	-0.220472
Cl_7	2.618814	1.668832	-0.327876
C_8	0.224108	1.194496	0.671052
O_9	0.510556	2.411620	1.201937
C_{10}	-0.953295	0.484952	0.928275
C_{11}	-1.156673	-0.692412	0.220472
Cl_{12}	-2.618814	-1.668832	0.327876
C_{13}	-0.224108	-1.194496	-0.671052
O_{14}	-0.510556	-2.411620	-1.201937
C_{15}	-1.893120	1.093499	1.904442
O_{16}	-1.669103	2.195561	2.414328
O_{17}	-2.995896	0.448861	2.195558
C_{18}	-4.041063	1.157649	2.929126
H_{19}	3.630559	-1.606146	-3.821157
H_{20}	4.773061	-0.403343	-3.164490
H_{21}	4.457586	-1.920722	-2.281094
H_{22}	-0.119312	2.711630	1.883639
H_{23}	0.119312	-2.711630	-1.883639
H_{24}	-3.630559	1.606146	3.821157
H_{25}	-4.773061	0.403343	3.164490
H_{26}	-4.457586	1.920722	2.281094

Table 10S: Cartesian coordinates for dimethyl 3,6-dichloro-2,5-dihydroxyterephthalate obtained using the PCX model (polarized basis set).

Atom	x-coordinate	y-coordinate	z-coordinate
C_1	4.014714	-1.194597	-2.867711
O_2	3.013082	-0.485048	-2.138626
C_3	1.929290	-1.134903	-1.873115
O_4	1.705898	-2.213296	-2.366714
C_5	0.967340	-0.507158	-0.904975
C_6	1.181010	0.665642	-0.181697
Cl_7	2.629967	1.568609	-0.241187
C_8	0.231431	1.194387	0.686041
O_9	0.526469	2.372038	1.231855
C_{10}	-0.967340	0.507158	0.904975
C_{11}	-1.181010	-0.665642	0.181697
Cl_{12}	-2.629967	-1.568609	0.241187
C_{13}	-0.231431	-1.194387	-0.686041
O_{14}	-0.526469	-2.372038	-1.231855
C_{15}	-1.929290	1.134903	1.873115
O_{16}	-1.705898	2.213296	2.366714
O_{17}	-3.013082	0.485048	2.138626
C_{18}	-4.014714	1.194597	2.867711
H_{19}	3.599702	-1.628293	-3.763695
H_{20}	4.771168	-0.464450	-3.112353
H_{21}	4.425732	-1.976173	-2.239229
H_{22}	-0.157769	2.637147	1.848877
H_{23}	0.157769	-2.637147	-1.848877
H_{24}	-3.599702	1.628293	3.763695
H_{25}	-4.771168	0.464450	3.112353
H_{26}	-4.425732	1.976173	2.239229

Table 11S: Cartesian coordinates for dimethyl 3,6-dichloro-2,5-dihydroxyterephthalate obtained using the SM model.

Atom	x-coordinate	y-coordinate	z-coordinate
C_1	4.158275	-1.274457	-2.722963
O_2	3.175534	-0.617182	-1.862017
C_3	1.931219	-1.024838	-1.902340
O_4	1.574720	-1.864703	-2.728343
C_5	0.973555	-0.466510	-0.911099
C_6	1.307860	0.398345	0.122526
Cl_7	2.968753	0.975556	0.404356
C_8	0.365064	0.871464	1.021230
O_9	0.822653	1.729930	1.969454
C_{10}	-0.973555	0.466510	0.911099
C_{11}	-1.307860	-0.398345	-0.122526
Cl_{12}	-2.968753	-0.975556	-0.404356
C_{13}	-0.365064	-0.871464	-1.021230
O_{14}	-0.822653	-1.729930	-1.969454
C_{15}	-1.931219	1.024838	1.902340
O_{16}	-1.574720	1.864703	2.728343
O_{17}	-3.175534	0.617182	1.862017
C_{18}	-4.158275	1.274457	2.722963
H_{19}	3.938181	-1.029992	-3.750864
H_{20}	5.105958	-0.872878	-2.403589
H_{21}	4.105183	-2.341620	-2.553885
H_{22}	0.131235	2.107652	2.547583
H_{23}	-0.131235	-2.107652	-2.547583
H_{24}	-3.938181	1.029992	3.750864
H_{25}	-5.105958	0.872878	2.403589
H_{26}	-4.105183	2.341620	2.553885

Table 12S: Cartesian coordinates for dimethyl 3,6-dichloro-2,5-dihydroxyterephthalate obtained using the SMX-15 model.

Atom	x-coordinate	y-coordinate	z-coordinate
C_1	4.118400	-1.275187	-2.777781
O_2	3.099046	-0.569274	-2.002170
C_3	1.954685	-1.170389	-1.784217
O_4	1.708829	-2.250833	-2.319742
C_5	0.981726	-0.527971	-0.866094
C_6	1.209359	0.631418	-0.143968
Cl_7	2.738524	1.539545	-0.231006
C_8	0.257142	1.167958	0.704751
O_9	0.601733	2.323159	1.331020
C_{10}	-0.981726	0.527971	0.866094
C_{11}	-1.209359	-0.631418	0.143968
Cl_{12}	-2.738524	-1.539545	0.231006
C_{13}	-0.257142	-1.167958	-0.704751
O_{14}	-0.601733	-2.323159	-1.331020
C_{15}	-1.954685	1.170389	1.784217
O_{16}	-1.708829	2.250833	2.319742
O_{17}	-3.099046	0.569274	2.002170
C_{18}	-4.118400	1.275187	2.777781
H_{19}	3.773219	-1.376737	-3.795257
H_{20}	4.991664	-0.647543	-2.705700
H_{21}	4.288935	-2.242548	-2.324583
H_{22}	-0.106787	2.727259	1.868948
H_{23}	0.106787	-2.727259	-1.868948
H_{24}	-3.773219	1.376737	3.795257
H_{25}	-4.991664	0.647543	2.705700
H_{26}	-4.288935	2.242548	2.324583

Table 13S: Cartesian coordinates for dimethyl 3,6-dichloro-2,5-dihydroxyterephthalate obtained using the SMX-11 model.

Atom	x-coordinate	y-coordinate	z-coordinate
C_1	4.102464	-1.209758	-2.833023
O_2	3.082202	-0.530527	-2.039110
C_3	1.954005	-1.154628	-1.798906
O_4	1.721665	-2.243332	-2.324617
C_5	0.980768	-0.522144	-0.871573
C_6	1.199846	0.647366	-0.159807
Cl_7	2.719215	1.570994	-0.261338
C_8	0.246278	1.179105	0.692050
O_9	0.579091	2.345868	1.303091
C_{10}	-0.980768	0.522144	0.871573
C_{11}	-1.199846	-0.647366	0.159807
Cl_{12}	-2.719215	-1.570994	0.261338
C_{13}	-0.246278	-1.179105	-0.692050
O_{14}	-0.579091	-2.345868	-1.303091
C_{15}	-1.954005	1.154628	1.798906
O_{16}	-1.721665	2.243332	2.324617
O_{17}	-3.082202	0.530527	2.039110
C_{18}	-4.102464	1.209758	2.833023
H_{19}	3.734859	-1.344357	-3.838312
H_{20}	4.951878	-0.546124	-2.804031
H_{21}	4.322252	-2.161983	-2.366722
H_{22}	-0.126332	2.739873	1.851355
H_{23}	0.126332	-2.739873	-1.851355
H_{24}	-3.734859	1.344357	3.838312
H_{25}	-4.951878	0.546124	2.804031
H_{26}	-4.322252	2.161983	2.366722

Table 14S: Cartesian coordinates for 2-(2-methyl-3-chloroanilino) nicotinic acid (NIC-I) obtained using the PCX model.

Atom	x-coordinate	y-coordinate	z-coordinate
N_1	3.543719	6.408743	2.000834
C_2	3.957482	7.610352	2.375497
C_3	3.449428	8.788249	1.762986
C_4	2.545912	8.635593	0.727462
C_5	2.147366	7.369526	0.321068
C_6	2.667145	6.297340	1.004020
N_7	4.901232	7.698047	3.352982
C_8	5.436148	6.628993	4.102989
C_9	6.276971	5.672592	3.517611
C_{10}	6.749975	4.669099	4.357514
C_{11}	6.503396	4.631540	5.715392
C_{12}	5.721417	5.625011	6.271928
C_{13}	5.174687	6.603956	5.467122
C_{14}	6.666176	5.749180	2.064144
C_{15}	3.800244	10.142833	2.255949
O_{16}	3.330302	11.106569	1.507069
O_{17}	4.424405	10.351196	3.260032
Cl_{18}	7.710797	3.349067	3.688929
H_{19}	2.142188	9.515784	0.258215
H_{20}	1.449323	7.224891	-0.484684
H_{21}	2.369699	5.287259	0.756563
H_{22}	5.034679	8.621230	3.722790
H_{23}	6.932599	3.856570	6.326744
H_{24}	5.546208	5.628011	7.335392
H_{25}	4.547696	7.372867	5.889745
H_{26}	6.038801	5.099450	1.455614
H_{27}	7.702457	5.453856	1.926155
H_{28}	6.547893	6.768198	1.711545
H_{29}	3.460111	11.961676	1.951629

Table 15S: Cartesian coordinates for 2-(2-methyl-3-chloroanilino) nicotinic acid (NIC-II) obtained using the PCX model.

Atom	x-coordinate	y-coordinate	z-coordinate
N_1	1.338987	1.077053	5.642450
C_2	2.536765	1.608827	5.806724
C_3	3.253043	2.175300	4.719854
C_4	2.655371	2.139671	3.465070
C_5	1.401547	1.576868	3.313344
C_6	0.787094	1.069099	4.439351
N_7	3.102683	1.576199	7.050295
C_8	2.570683	1.163025	8.274481
C_9	3.499803	0.864720	9.292231
C_{10}	2.983598	0.509514	10.527430
C_{11}	1.626805	0.415566	10.782433
C_{12}	0.743275	0.703397	9.766672
C_{13}	1.204876	1.077320	8.520364
C_{14}	4.982988	0.952190	9.022912
C_{15}	4.593836	2.772058	4.862316
O_{16}	4.937079	3.505411	3.839939
O_{17}	5.322949	2.631503	5.820329
Cl_{18}	4.051622	0.152999	11.861078
H_{19}	3.188261	2.535195	2.614944
H_{20}	0.915712	1.538259	2.353009
H_{21}	-0.200627	0.630988	4.387039
H_{22}	4.025127	1.954508	7.082452
H_{23}	1.288267	0.110748	11.758189
H_{24}	-0.320157	0.648071	9.947834
H_{25}	0.523062	1.295572	7.726776
H_{26}	5.318283	1.987229	8.981896
H_{27}	5.229645	0.488432	8.071326
H_{28}	5.565699	0.460991	9.789631
H_{29}	5.847988	3.816070	3.904927

Table 16S: Cartesian coordinates for 2-(2-methyl-3-chloroanilino) nicotinic acid (NIC-III) obtained using the PCX model.

Atom	x-coordinate	y-coordinate	z-coordinate
N_1	4.305810	1.042482	3.001136
C_2	3.288453	1.425244	3.747708
C_3	2.036359	1.768944	3.168274
C_4	1.912062	1.677039	1.790635
C_5	2.989005	1.272801	1.022662
C_6	4.156208	0.977042	1.685967
N_7	3.442366	1.511065	5.104318
C_8	4.520124	1.234502	5.939107
C_9	4.295131	1.433438	7.324329
C_{10}	5.365088	1.205914	8.170882
C_{11}	6.609729	0.776115	7.739913
C_{12}	6.795647	0.580209	6.393163
C_{13}	5.768006	0.811069	5.492898
C_{14}	2.929539	1.856987	7.810990
C_{15}	0.898013	2.260310	3.967009
O_{16}	-0.176987	2.487672	3.266865
O_{17}	0.938674	2.452622	5.160280
Cl_{18}	5.208637	1.477153	9.897574
H_{19}	0.975940	1.939766	1.328349
H_{20}	2.929418	1.215542	-0.049225
H_{21}	5.037733	0.688596	1.133122
H_{22}	2.604506	1.806227	5.558141
H_{23}	7.401445	0.613123	8.448949
H_{24}	7.756286	0.252324	6.031109
H_{25}	5.924225	0.680735	4.444428
H_{26}	2.188025	1.105392	7.546154
H_{27}	2.611118	2.792491	7.356973
H_{28}	2.906061	1.996457	8.882860
H_{29}	-0.853842	2.898057	3.820006

Table 17S: Cartesian coordinates for 2-(2-methyl-3-chloroanilino) nicotinic acid (NIC-IV) obtained using the PCX model.

Atom	x-coordinate	y-coordinate	z-coordinate
N_1	5.875943	0.255843	7.249455
C_2	6.426620	-0.466132	6.259304
C_3	5.544528	-1.075460	5.312251
C_4	4.207646	-0.849684	5.435351
C_5	3.665982	-0.060942	6.484432
C_6	4.525129	0.459177	7.374286
N_7	7.742732	-0.641157	6.146546
C_8	8.795857	-0.046091	6.874953
C_9	9.862949	0.550739	6.181559
C_{10}	10.886763	1.063676	6.973571
C_{11}	10.875883	1.031530	8.355075
C_{12}	9.822322	0.422649	9.000012
C_{13}	8.801045	-0.134518	8.257773
C_{14}	9.934140	0.608919	4.674875
C_{15}	6.066325	-1.912782	4.138450
O_{16}	5.215065	-2.520039	3.502276
O_{17}	7.293350	-1.921310	3.973262
Cl_{18}	12.285264	1.785039	6.215271
H_{19}	6.436686	0.675172	7.986397
H_{20}	3.553830	-1.294551	4.703063
H_{21}	2.604693	0.111781	6.555886
H_{22}	4.246881	1.060719	8.224479
H_{23}	7.943572	-1.142853	5.271994
H_{24}	11.687701	1.470912	8.908908
H_{25}	9.822040	0.361421	10.077487
H_{26}	7.998777	-0.663179	8.739784
H_{27}	10.793790	0.044208	4.323322
H_{28}	10.045603	1.635040	4.336811
H_{29}	9.041488	0.214250	4.211474

Table 18S: MM parameters for formamide oxime.

Atom	Atom type	Charge
C_1	CN4	0.53
N_2	NN1	-0.68
N_3	NN4	-0.60
O_4	OH1	-0.54
H_5	HN1	0.32
H_6	HN1	0.36
H_7	HN3	0.18
H_8	H	0.43

Table 19S: MM parameters for dimethyl 3,6-dichloro-2,5-dihydroxyterephthalate.

Atom	Atom type	Charge
C_1	CT3	-0.14
O_2	OS	-0.34
C_3	CD	0.63
O_4	OB	-0.52
C_5	CA	0.10
C_6	CA	0.12
Cl_7	CL	-0.12
C_8	CA	0.11
O_9	OH1	-0.54
C_{10}	CA	0.10
C_{11}	CA	0.12
Cl_{12}	CL[a]	-0.12
C_{13}	CA	0.11
O_{14}	OH1	-0.54
C_{15}	CD	0.63
O_{16}	OB	-0.52
O_{17}	OS	-0.34
C_{18}	CT3	-0.14
H_{19}	HA	0.09
H_{20}	HA	0.09
H_{21}	HA	0.09
H_{22}	H	0.43
H_{23}	H	0.43
H_{24}	HA	0.09
H_{25}	HA	0.09
H_{26}	HA	0.09

[a] Van der Waals parameters: 0.00, -0.30, 2.27

Table 20S: MM parameters for 2-(2-methyl-3-chloroanilino) nicotinic acid (NIC-I, NIC-II, and NIC-III).

Atom	Atom type	Charge
N_1	NN3G	-0.74
C_2	CN2	0.47
C_3	CN3	0.05
C_4	CN3A	-0.05
C_5	CN3	-0.10
C_6	CN3B	0.16
N_7	NH1	-0.47
C_8	CPT	0.13
C_9	CPT	-0.02
C_{10}	CPT	0.13
C_{11}	CA	-0.12
C_{12}	CA	-0.12
C_{13}	CA	-0.12
C_{14}	CN9	-0.11
C_{15}	CD	0.75
O_{16}	OH1	-0.61
O_{17}	OB	-0.55
Cl_{18}	CL[a]	-0.48
H_{19}	HN3B	0.16
H_{20}	HN3B	0.16
H_{21}	HN3B	0.16
H_{22}	H	0.31
H_{23}	HP	0.12
H_{24}	HP	0.12
H_{25}	HP	0.12
H_{26}	HN9	0.07
H_{27}	HN9	0.07
H_{28}	HN9	0.07
H_{29}	H	0.44

[a] Van der Waals parameters: 0.00, -0.30, 2.27

Table 21S: MM parameters for 2-(2-methyl-3-chloroanilino) nicotinic acid (NIC-IV).

Atom	Atom type	Charge
N_1	NN2	-0.52
C_2	CN2	0.73
C_3	CN3	0.05
C_4	CN3A	-0.05
C_5	CN3	-0.10
C_6	CN3B	0.16
N_7	NH1	-0.47
C_8	CPT	0.13
C_9	CPT	-0.02
C_{10}	CPT	0.13
C_{11}	CA	-0.12
C_{12}	CA	-0.12
C_{13}	CA	-0.12
C_{14}	CN9	-0.11
C_{15}	CC	0.62
O_{16}	OC	-0.76
O_{17}	OC	-0.76
Cl_{18}	CL[a]	-0.48
H_{19}	HN2	0.45
H_{20}	HN3B	0.16
H_{21}	HN3B	0.16
H_{22}	HN3B	0.16
H_{23}	H	0.31
H_{24}	HP	0.12
H_{25}	HP	0.12
H_{26}	HP	0.12
H_{27}	HN9	0.07
H_{28}	HN9	0.07
H_{29}	HN9	0.07

[a] Van der Waals parameters: 0.00, -0.30, 2.27