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APPENDIXES

APPENDIX I : NUMERICAL RADIAL DISTRIBUTION FUNCTIONS OBTAINED FROM MONTE CARLO SIMULATION (R IS GIVEN IN Å)

A. Lithium(I)/water radial distribution function

R	g(LO)	INT(LO)	g(LH)	INT(LH)	R	g(LO)	INT(LO)	g(LH)	INT(LH)
0.00000	0.00000	0.00000	0.00000	0.00000	1.75000	2.25725	0.14847	0.00000	0.00000
0.05000	0.00000	0.00000	0.00000	0.00000	1.80000	5.07067	0.41299	0.00000	0.00000
0.10000	0.00000	0.00000	0.00000	0.00000	1.85000	8.79778	0.89779	0.00000	0.00000
0.15000	0.00000	0.00000	0.00000	0.00000	1.90000	11.29313	1.55418	0.00000	0.00000
0.20000	0.00000	0.00000	0.00000	0.00000	1.95000	11.58751	2.26361	0.00000	0.00000
0.25000	0.00000	0.00000	0.00000	0.00000	2.00000	9.59611	2.88163	0.00000	0.00000
0.30000	0.00000	0.00000	0.00000	0.00000	2.05000	6.82604	3.34350	0.00522	0.00035
0.35000	0.00000	0.00000	0.00000	0.00000	2.10000	4.00277	3.62771	0.02916	0.00242
0.40000	0.00000	0.00000	0.00000	0.00000	2.15000	2.26221	3.79608	0.09839	0.00975
0.45000	0.00000	0.00000	0.00000	0.00000	2.20000	1.04204	3.87728	0.23783	0.02828
0.50000	0.00000	0.00000	0.00000	0.00000	2.25000	0.53653	3.92101	0.50432	0.06939
0.55000	0.00000	0.00000	0.00000	0.00000	2.30000	0.20278	3.93828	0.88759	0.14499
0.60000	0.00000	0.00000	0.00000	0.00000	2.35000	0.09996	3.94717	1.40113	0.26957
0.65000	0.00000	0.00000	0.00000	0.00000	2.40000	0.06643	3.95333	2.11659	0.46586
0.70000	0.00000	0.00000	0.00000	0.00000	2.45000	0.04912	3.95808	2.83996	0.74033
0.75000	0.00000	0.00000	0.00000	0.00000	2.50000	0.04115	3.96222	3.47624	1.09014
0.80000	0.00000	0.00000	0.00000	0.00000	2.55000	0.01833	3.96414	3.96012	1.50475
0.85000	0.00000	0.00000	0.00000	0.00000	2.60000	0.01856	3.96616	4.28810	1.97147
0.90000	0.00000	0.00000	0.00000	0.00000	2.65000	0.02323	3.96878	4.06483	2.43107
0.95000	0.00000	0.00000	0.00000	0.00000	2.70000	0.03098	3.97242	3.79004	2.87592
1.00000	0.00000	0.00000	0.00000	0.00000	2.75000	0.02571	3.97555	3.11224	3.25487
1.05000	0.00000	0.00000	0.00000	0.00000	2.80000	0.03521	3.97999	2.30877	3.54631
1.10000	0.00000	0.00000	0.00000	0.00000	2.85000	0.05252	3.98686	1.60059	3.75563
1.15000	0.00000	0.00000	0.00000	0.00000	2.90000	0.05594	3.99443	0.97753	3.88799
1.20000	0.00000	0.00000	0.00000	0.00000	2.95000	0.10236	4.00877	0.60261	3.97242
1.25000	0.00000	0.00000	0.00000	0.00000	3.00000	0.13452	4.02827	0.41646	4.03277
1.30000	0.00000	0.00000	0.00000	0.00000	3.05000	0.17330	4.05422	0.31323	4.07968
1.35000	0.00000	0.00000	0.00000	0.00000	3.10000	0.17559	4.08139	0.25719	4.11948
1.40000	0.00000	0.00000	0.00000	0.00000	3.15000	0.22317	4.11704	0.28291	4.16467
1.45000	0.00000	0.00000	0.00000	0.00000	3.20000	0.25513	4.15977	0.30385	4.21477
1.50000	0.00000	0.00000	0.00000	0.00000	3.25000	0.33317	4.21643	0.33080	4.27103
1.55000	0.00000	0.00000	0.00000	0.00000	3.30000	0.41647	4.28945	0.32776	4.32849
1.60000	0.00245	0.00010	0.00000	0.00000	3.35000	0.44158	4.36924	0.33314	4.38869
1.65000	0.10829	0.00485	0.00000	0.00000	3.40000	0.51117	4.46438	0.34214	4.45237
1.70000	0.69459	0.03717	0.00000	0.00000	3.45000	0.52176	4.56437	0.34073	4.51767

A. Lithium(I)/water radial distribution function

R	g(LO)	INT(LO)	g(LH)	INT(LH)	R	g(LO)	INT(LO)	g(LH)	INT(LH)
3.50000	0.54076	4.67102	0.37075	4.59079	5.40000	0.98656	15.32649	0.99064	15.59325
3.55000	0.56346	4.78536	0.36511	4.66487	5.45000	0.98923	15.79957	0.97530	16.05966
3.60000	0.59148	4.90878	0.42086	4.75269	5.50000	1.05490	16.31335	0.97278	16.53345
3.65000	0.61117	5.03988	0.43178	4.84531	5.55000	1.08648	16.85219	0.96633	17.01268
3.70000	0.62547	5.17774	0.47059	4.94903	5.60000	1.13678	17.42616	0.95195	17.49333
3.75000	0.61693	5.31742	0.47284	5.05609	5.65000	1.20989	18.04800	0.95571	17.98454
3.80000	0.62165	5.46195	0.50653	5.17386	5.70000	1.18818	18.66956	0.97792	18.49609
3.85000	0.65978	5.61941	0.53155	5.30072	5.75000	1.18260	19.29909	0.98945	19.02280
3.90000	0.66029	5.78111	0.54213	5.43348	5.80000	1.21693	19.95821	0.97023	19.54829
3.95000	0.69635	5.95604	0.54478	5.57033	5.85000	1.23948	20.64116	0.98817	20.09277
4.00000	0.79079	6.15976	0.55947	5.71446	5.90000	1.22955	21.33028	1.00465	20.65584
4.05000	0.88459	6.39337	0.59814	5.87242	5.95000	1.20702	22.01828	1.04064	21.24901
4.10000	0.98704	6.66051	0.62245	6.04089	6.00000	1.12949	22.67296	1.02999	21.84601
4.15000	1.05154	6.95210	0.64961	6.22102	6.05000	1.04354	23.28793	1.03317	22.45488
4.20000	1.11413	7.26853	0.65539	6.40717	6.10000	1.03510	23.90807	1.01605	23.06360
4.25000	1.13426	7.59840	0.69546	6.60942	6.15000	1.05582	24.55103	1.03385	23.69318
4.30000	1.18878	7.95230	0.71738	6.82298	6.20000	1.00541	25.17328	1.01512	24.32144
4.35000	1.22891	8.32671	0.72385	7.04352	6.25000	1.00962	25.80826	1.01283	24.95844
4.40000	1.22868	8.70970	0.74751	7.27652	6.30000	0.98844	26.43991	1.01357	25.60614
4.45000	1.23892	9.10471	0.76882	7.52165	6.35000	0.96983	27.06953	1.02327	26.27046
4.50000	1.16879	9.48578	0.80728	7.78486	6.40000	0.97357	27.71158	1.02694	26.94771
4.55000	1.15355	9.87029	0.87387	8.07614	6.45000	0.99020	28.37483	1.05790	27.65631
4.60000	1.00617	10.21308	0.94110	8.39676	6.50000	1.02491	29.07202	1.08237	28.39259
4.65000	0.91241	10.53072	0.97246	8.73531	6.55000	1.02336	29.77892	1.09530	29.14917
4.70000	0.79087	10.81201	1.03807	9.10452	6.60000	1.00892	30.48651	1.08719	29.91167
4.75000	0.73149	11.07774	1.08598	9.49902	6.65000	1.01863	31.21178	1.07771	30.67900
4.80000	0.70054	11.33761	1.10445	9.90873	6.70000	1.00893	31.94099	1.07042	31.45265
4.85000	0.67017	11.59142	1.12006	10.33293	6.75000	1.02942	32.69617	1.05572	32.22711
4.90000	0.64585	11.84109	1.15336	10.77879	6.80000	0.99793	33.43912	1.05416	33.01192
4.95000	0.61443	12.08349	1.16192	11.23718	6.85000	1.03876	34.22388	1.05113	33.80602
5.00000	0.64035	12.34124	1.18008	11.71218	6.90000	1.05235	35.03055	1.05703	34.61627
5.05000	0.69414	12.62626	1.16839	12.19193	6.95000	1.07415	35.86591	1.02441	35.41295
5.10000	0.73896	12.93573	1.15777	12.67678	7.00000	1.09214	36.72752	1.01776	36.21590
5.15000	0.76537	13.26256	1.16330	13.17355	7.05000	1.06169	37.57713	1.03272	37.04233
5.20000	0.84351	13.62980	1.13965	13.66971	7.10000	1.01791	38.40331	1.03453	37.88199
5.25000	0.87645	14.01875	1.12317	14.16814	7.15000	0.99759	39.22443	1.05152	38.74750
5.30000	0.90399	14.42759	1.07349	14.65365	7.20000	0.95499	40.02151	1.08537	39.65341
5.35000	0.94547	14.86331	1.02963	15.12815	7.25000	0.96394	40.83728	1.10458	40.58821

A. Lithium(I)/water radial distribution function

R	g(LO)	INT(LO)	g(LH)	INT(LH)	R	g(LO)	INT(LO)	g(LH)	INT(LH)
7.30000	0.98468	41.68213	1.10240	41.53407	8.70000	0.91524	69.82260	0.89533	69.01440
7.35000	1.01731	42.56699	1.09012	42.48225	8.75000	0.91218	70.87309	0.90238	70.10211
7.40000	1.07956	43.51880	1.05745	43.41458	8.80000	0.91873	71.94379	0.91230	71.18973
7.45000	1.09902	44.50092	1.04274	44.34641	8.85000	0.91157	73.05548	0.91577	72.29410
7.50000	1.12992	45.52423	1.03864	45.28706	8.90000	0.90577	74.19788	0.91779	73.41357
7.55000	1.15726	46.58633	1.02080	46.22394	8.95000	0.91727	75.38087	0.91417	74.56679
7.60000	1.16717	47.67177	0.99590	47.15010	9.00000	0.91524	69.82260	0.89533	69.01440
7.65000	1.18123	48.78477	1.01969	48.11090	9.05000	0.91218	70.87309	0.90238	70.10211
7.70000	1.18752	49.91840	1.02363	49.08807	9.10000	0.91873	71.94379	0.91230	71.18973
7.75000	1.15157	51.03201	1.01778	50.07231	9.15000	0.91157	73.05548	0.91577	72.29410
7.80000	1.12901	52.13795	1.02441	51.07579	9.20000	0.91577	74.19788	0.91779	73.41357
7.85000	1.09585	53.22520	1.02718	52.09492	9.25000	0.91727	74.38087	0.91417	74.56679
7.90000	1.03548	54.26570	1.00322	53.10300	9.30000	0.91524	74.82260	0.89533	69.01440
7.95000	0.99659	55.27983	0.97530	54.09546	9.35000	0.91218	74.87309	0.90238	70.10211
8.00000	0.93370	56.24194	0.96384	55.08864	9.40000	0.91873	74.94379	0.91230	71.18973
8.05000	0.92078	57.20265	0.93341	56.06252	9.45000	0.91157	75.05548	0.91577	72.29410
8.10000	0.89013	58.14296	0.91604	57.03018	9.50000	0.91577	75.08788	0.91779	73.41357
8.15000	0.85790	59.06044	0.88718	57.97897	9.55000	0.91727	75.38087	0.91417	74.56679
8.20000	0.85036	59.98105	0.87798	58.92947	9.60000	0.91524	69.82260	0.90533	69.01440
8.25000	0.86912	60.93347	0.85506	59.86650	9.65000	0.91218	70.87309	0.90238	70.10211
8.30000	0.84802	61.87407	0.85012	60.80943	9.70000	0.91873	71.94379	0.91230	71.18973
8.35000	0.86030	62.83983	0.84973	61.76332	9.75000	0.91157	73.05548	0.91577	72.29410
8.40000	0.84840	63.80367	0.84987	62.72882	9.80000	0.91577	74.19788	0.91779	73.41357
8.45000	0.86677	64.80013	0.86453	63.72270	9.85000	0.91727	75.38087	0.91517	74.56679
8.50000	0.86554	65.80699	0.87796	64.74400	9.90000	0.91157	73.05548	0.91577	72.29410
8.55000	0.87571	66.81415	0.88900	65.79036	9.95000	0.91577	74.19788	0.91779	73.41357
8.60000	0.89739	67.81131	0.88124	66.83974	10.00000	0.91727	75.38087	0.91617	74.56679
8.65000	0.90463	68.80473	0.89946	67.92331					

B. Lithium(I)/ammonia radial distribution function

R	g(LN)	INT(LN)	g(LH)	INT(LH)	R	g(LN)	INT(LN)	g(LH)	INT(LH)
0.00000	0.00000	0.00000	0.00000	0.00000	0.30000	0.00000	0.00000	0.00000	0.00000
0.05000	0.00000	0.00000	0.00000	0.00000	0.35000	0.00000	0.00000	0.00000	0.00000
0.10000	0.00000	0.00000	0.00000	0.00000	0.40000	0.00000	0.00000	0.00000	0.00000
0.15000	0.00000	0.00000	0.00000	0.00000	0.45000	0.00000	0.00000	0.00000	0.00000
0.20000	0.00000	0.00000	0.00000	0.00000	0.50000	0.00000	0.00000	0.00000	0.00000
0.25000	0.00000	0.00000	0.00000	0.00000	0.55000	0.00000	0.00000	0.00000	0.00000

B. Lithium(I)/ammonia radial distribution function

R	g(LN)	INT(LN)	g(LH)	INT(LH)	R	g(LN)	INT(LN)	g(LH)	INT(LH)
0.60000	0.00000	0.00000	0.00000	0.00000	2.50000	2.26887	0.18382	0.10189	0.01808
0.65000	0.00000	0.00000	0.00000	0.00000	2.55000	2.17249	0.23684	0.24139	0.03575
0.70000	0.00000	0.00000	0.00000	0.00000	2.60000	1.89868	0.28502	0.37814	0.06454
0.75000	0.00000	0.00000	0.00000	0.00000	2.65000	1.78556	0.33209	0.52749	0.10625
0.80000	0.00000	0.00000	0.00000	0.00000	2.70000	1.50965	0.37340	0.76528	0.16907
0.85000	0.00000	0.00000	0.00000	0.00000	2.75000	1.47660	0.41531	0.98677	0.25311
0.90000	0.00000	0.00000	0.00000	0.00000	2.80000	1.44836	0.45793	1.29048	0.36703
0.95000	0.00000	0.00000	0.00000	0.00000	2.85000	1.33173	0.49854	1.56693	0.51035
1.00000	0.00000	0.00000	0.00000	0.00000	2.90000	1.36939	0.54176	1.67974	0.66943
1.05000	0.00000	0.00000	0.00000	0.00000	2.95000	1.62328	0.59479	1.73459	0.83941
1.10000	0.00000	0.00000	0.00000	0.00000	3.00000	1.68921	0.65185	1.99118	1.04121
1.15000	0.00000	0.00000	0.00000	0.00000	3.05000	1.66032	0.70983	2.12698	1.26401
1.20000	0.00000	0.00000	0.00000	0.00000	3.10000	1.67719	0.77033	2.15599	1.49732
1.25000	0.00000	0.00000	0.00000	0.00000	3.15000	1.77081	0.83628	2.21102	1.74437
1.30000	0.00000	0.00000	0.00000	0.00000	3.20000	1.87619	0.90839	2.20465	1.99858
1.35000	0.00000	0.00000	0.00000	0.00000	3.25000	1.93100	0.98495	2.15263	2.25462
1.40000	0.00000	0.00000	0.00000	0.00000	3.30000	2.10766	1.07110	2.12907	2.51570
1.45000	0.00000	0.00000	0.00000	0.00000	3.35000	2.12194	1.16049	1.97328	2.76507
1.50000	0.00000	0.00000	0.00000	0.00000	3.40000	1.90403	1.24310	1.88386	3.01029
1.55000	0.00000	0.00000	0.00000	0.00000	3.45000	1.96906	1.33108	1.71888	3.24067
1.60000	0.00000	0.00000	0.00000	0.00000	3.50000	1.91540	1.41915	1.67524	3.47176
1.65000	0.00000	0.00000	0.00000	0.00000	3.55000	1.88745	1.50843	1.68603	3.71103
1.70000	0.00000	0.00000	0.00000	0.00000	3.60000	1.65890	1.58913	1.66444	3.95393
1.75000	0.00000	0.00000	0.00000	0.00000	3.65000	1.43401	1.66084	1.55182	4.13674
1.80000	0.00000	0.00000	0.00000	0.00000	3.70000	1.37782	1.73164	1.45055	4.41035
1.85000	0.00000	0.00000	0.00000	0.00000	3.75000	1.34707	1.80274	1.41467	4.63437
1.90000	0.00000	0.00000	0.00000	0.00000	3.80000	1.25781	1.87092	1.39633	4.85141
1.95000	0.00000	0.00000	0.00000	0.00000	3.85000	1.31430	1.94404	1.26045	5.07180
2.00000	0.00000	0.00000	0.00000	0.00000	3.90000	1.32859	2.01989	1.22244	5.23117
2.05000	0.00000	0.00000	0.00000	0.00000	3.95000	1.46762	2.10584	1.18019	5.43852
2.10000	0.01220	0.00020	0.00000	0.00000	4.00000	1.65820	2.20543	1.10266	5.63719
2.15000	0.04657	0.00101	0.00000	0.00000	4.05000	1.75039	2.31319	1.14177	5.83808
2.20000	0.18346	0.00434	0.00000	0.00000	4.10000	1.99768	2.43924	1.09008	6.10442
2.25000	0.33485	0.01071	0.00709	0.00040	4.15000	2.13576	2.57731	1.14001	6.32551
2.30000	0.74264	0.02545	0.02204	0.00172	4.20000	2.34757	2.73274	1.06879	6.53781
2.35000	1.31555	0.05272	0.02599	0.00333	4.25000	2.41333	2.89636	1.15701	6.77314
2.40000	1.63035	0.08797	0.04360	0.00616	4.30000	2.60347	3.07705	1.19720	7.02240
2.45000	1.89173	0.13059	0.07023	0.01091	4.35000	2.71603	3.26996	1.32720	7.30520

B. Lithium(I)/ammonia radial distribution function

R	g(LN)	INT(LN)	g(LH)	INT(LH)	R	g(LN)	INT(LN)	g(LH)	INT(LH)
4.40000	3.11887	3.49660	1.38338	7.60679	6.30000	1.31658	8.82827	1.10596	24.05200
4.45000	3.40382	3.74961	1.44713	7.92948	6.35000	1.26857	9.02027	1.17715	24.58649
4.50000	3.53722	4.01847	1.48203	8.26743	6.40000	1.22912	9.20924	1.14306	25.11369
4.55000	3.46771	4.28794	1.57615	8.63486	6.45000	1.13446	9.38640	1.15731	25.65585
4.60000	3.01760	4.52761	1.62558	9.02220	6.50000	1.11516	9.56325	1.14870	26.20236
4.65000	2.87092	4.76062	1.73972	9.44579	6.55000	1.06559	9.73484	1.16824	26.76674
4.70000	2.59699	4.97595	1.84583	9.90493	6.60000	1.04395	9.90553	1.18684	27.34889
4.75000	2.33748	5.17391	1.98765	10.40993	6.65000	1.05569	10.08077	1.18630	27.93964
4.80000	1.98305	5.34540	2.08038	10.94967	6.70000	1.05617	10.25873	1.20563	28.54906
4.85000	1.58776	5.48559	2.16468	11.52305	6.75000	1.15693	10.45659	1.19531	29.16232
4.90000	1.24845	5.59810	2.17265	12.11046	6.80000	1.15569	10.65717	1.17082	29.77196
4.95000	0.98725	5.68890	2.14289	12.70172	6.85000	1.12569	10.85543	1.17577	30.39320
5.00000	0.66193	5.75102	2.05612	13.28055	6.90000	1.12243	11.05602	1.14692	31.00809
5.05000	0.55499	5.80414	1.93682	13.83675	6.95000	1.10133	11.25570	1.14273	31.62964
5.10000	0.48209	5.85121	1.85558	14.38023	7.00000	1.10761	11.45941	1.07155	32.22089
5.15000	0.38856	5.88989	1.70678	14.88998	7.05000	1.16613	11.67697	1.01563	32.78931
5.20000	0.35227	5.92564	1.58555	15.37276	7.10000	1.08464	11.88220	0.97628	33.34349
5.25000	0.41198	5.96827	1.49138	15.83564	7.15000	1.06637	12.08682	0.96776	33.90060
5.30000	0.41669	6.01220	1.41644	16.28366	7.20000	1.04486	12.29013	0.95870	34.46024
5.35000	0.54808	6.07108	1.26662	16.69189	7.25000	1.06224	12.49971	0.95934	35.02805
5.40000	0.62840	6.13986	1.19960	17.08578	7.30000	1.05127	12.70999	0.92184	35.58121
5.45000	0.64229	6.21147	1.03002	17.43028	7.35000	1.03054	12.91896	0.87763	36.11508
5.50000	0.70628	6.29167	0.95653	17.75610	7.40000	0.95180	13.11460	0.83436	36.62956
5.55000	0.82027	6.38650	0.94694	18.08455	7.45000	0.94343	13.31114	0.82788	37.14697
5.60000	0.91724	6.49447	0.86146	18.38875	7.50000	0.96677	13.51526	0.80795	37.65874
5.65000	1.02835	6.61769	0.84094	18.69104	7.55000	0.93796	13.71595	0.77699	38.15747
5.70000	1.08824	6.75041	0.85386	19.00342	7.60000	0.99926	13.93259	0.77518	38.66165
5.75000	1.13043	6.89069	0.87543	19.32933	7.65000	0.87635	14.12510	0.76600	39.16644
5.80000	1.21501	7.04411	0.90439	19.67192	7.70000	0.84958	14.31417	0.78090	39.68779
5.85000	1.16839	7.19420	0.93198	20.03107	7.75000	0.79878	14.49425	0.81670	40.24016
5.90000	1.24916	7.35741	0.97990	20.41516	7.80000	0.75098	14.66575	0.85521	40.82605
5.95000	1.26397	7.52538	0.99694	20.81259	7.85000	0.77114	14.84411	0.87229	41.43134
6.00000	1.38276	7.71222	1.05887	21.24184	7.90000	0.81357	15.03470	0.89980	42.06369
6.05000	1.30928	7.89211	1.06374	21.68027	7.95000	0.85531	15.23761	0.91137	42.71230
6.10000	1.28284	8.07128	1.08591	22.13527	8.00000	0.87493	15.44779	0.93687	43.38747
6.15000	1.32467	8.25934	1.08231	22.59622	8.05000	0.85869	15.65666	0.92388	44.06163
6.20000	1.31249	8.44871	1.08266	23.06485	8.10000	0.81080	15.85633	0.92495	44.74498
6.25000	1.25093	8.63213	1.12051	23.55772	8.15000	0.87259	16.07388	0.93767	45.44632

B. Lithium(I)/ammonia radial distribution function

R	g(LN)	INT(LN)	g(LH)	INT(LH)
8.20000	0.87198	16.29396	0.92894	46.14967
8.25000	0.87686	16.51797	0.94289	46.87231
8.30000	0.91867	16.75552	0.91450	47.58173
8.35000	0.91542	16.99509	0.89021	48.28064
8.40000	0.89388	17.23183	0.83146	48.94127
8.45000	0.88333	17.46857	0.81135	49.59361
8.50000	0.84988	17.69904	0.76422	50.21536
8.55000	0.82046	17.92416	0.73494	50.82034
8.60000	0.80913	18.14877	0.70101	51.39583
8.65000	0.81239	18.37692	0.73585	51.96526
8.70000	0.83975	18.58992	0.76244	52.50429
8.75000	0.84657	18.79010	0.83519	53.05190
8.80000	0.85011	18.97906	0.86170	53.57658
8.85000	0.84156	19.15591	0.89274	54.09935
8.90000	0.85790	19.31287	0.90448	54.62959
8.95000	0.86007	19.52194	0.91774	55.15973
9.00000	0.86307	19.73194	0.91774	55.15973
9.05000	0.86427	19.94294	0.91784	55.18973
9.10000	0.86407	20.15334	0.91794	55.19973
9.15000	0.86507	20.37394	0.91804	55.20973
9.20000	0.86517	20.58344	0.91834	55.21973
9.25000	0.86607	20.71494	0.91804	55.22973
9.30000	0.86627	20.92424	0.91854	55.25973
9.35000	0.86637	21.03434	0.91874	55.28973
9.40000	0.86627	21.24424	0.91904	55.25973
9.45000	0.86657	21.46545	0.91934	55.30973
9.50000	0.86687	21.68194	0.91944	55.32973
9.55000	0.86707	21.80545	0.92054	55.30973
9.60000	0.86727	22.02294	0.92074	55.38973
9.65000	0.86767	22.25594	0.92174	55.40973
9.70000	0.86807	22.47894	0.92244	55.42973
9.75000	0.86827	22.71194	0.92204	55.45973
9.80000	0.86816	22.93194	0.92224	55.47973
9.85000	0.86837	23.29994	0.92254	55.48973
9.90000	0.86224	23.48194	0.92304	55.49973
9.95000	0.86221	23.63194	0.92314	55.50543
10.00000	0.86224	24.00094	0.92354	55.50673

C. Water/water radial distribution function

R	g(OO)	INT(OO)	g(OH)	INT(OH)	g(HH)	INT(HH)
1.90000	0.00000	0.00000	1.08309	0.46077	0.04064	0.00787
1.95000	0.00000	0.00000	1.08171	0.59322	0.08268	0.01800
2.00000	0.00000	0.00000	1.01793	0.72434	0.15337	0.03775
2.05000	0.00000	0.00000	0.91211	0.84777	0.25883	0.07278
2.10000	0.00000	0.00000	0.79544	0.96073	0.39774	0.12926
2.15000	0.00000	0.00000	0.68679	1.06296	0.56986	0.21408
2.20000	0.00000	0.00000	0.58122	1.15355	0.75374	0.33156
2.25000	0.00005	0.00000	0.49136	1.23365	0.93541	0.48405
2.30000	0.00029	0.00003	0.42474	1.30600	1.10007	0.67144
2.35000	0.00259	0.00026	0.37161	1.37208	1.23368	0.89083
2.40000	0.01455	0.00161	0.33363	1.43396	1.32294	1.13621
2.45000	0.05845	0.00726	0.30807	1.49351	1.37667	1.40230
2.50000	0.17939	0.02531	0.29338	1.55256	1.38800	1.68165
2.55000	0.41450	0.06871	0.28951	1.61318	1.36037	1.96650
2.60000	0.78646	0.15431	0.29470	1.67732	1.30169	2.24985
2.65000	1.26601	0.29745	0.31417	1.74837	1.23194	2.52843
2.70000	1.76146	0.50420	0.34662	1.82974	1.15324	2.79916
2.75000	2.15353	0.76642	0.39391	1.92566	1.07231	3.06029
2.80000	2.37553	1.06628	0.46113	2.04208	1.00073	3.31293
2.85000	2.42477	1.38339	0.54792	2.18539	0.94345	3.55970
2.90000	2.31752	1.69720	0.65613	2.36308	0.89336	3.80163
2.95000	2.12623	1.99512	0.77938	2.58149	0.85904	4.04236
3.00000	1.88876	2.26881	0.91667	2.84715	0.83286	4.28373
3.05000	1.64812	2.51566	1.06278	3.16551	0.81926	4.52915
3.10000	1.44928	2.73991	1.20827	3.53942	0.81400	4.78104
3.15000	1.27562	2.94370	1.33569	3.96620	0.81682	5.04203
3.20000	1.13832	3.13137	1.44522	4.44275	0.82458	5.31393
3.25000	1.04078	3.30837	1.51926	4.95949	0.83647	5.59844
3.30000	0.96816	3.47813	1.56010	5.50658	0.85580	5.89854
3.35000	0.91695	3.64381	1.57131	6.07442	0.87831	6.21595
3.40000	0.87990	3.80758	1.55542	6.65342	0.90524	6.55292
3.45000	0.85636	3.97169	1.51168	7.23282	0.93783	6.91237
3.50000	0.83973	4.13731	1.45393	7.80635	0.97016	7.29507
3.55000	0.83305	4.30634	1.38698	8.36921	1.00847	7.70433
3.60000	0.83509	4.48060	1.31621	8.91851	1.04599	8.14085
3.65000	0.84099	4.66099	1.24740	9.45364	1.08133	8.60475
3.70000	0.84654	4.84759	1.18568	9.97634	1.10882	9.09356
3.75000	0.85535	5.04125	1.13255	10.48919	1.13264	9.60645

C. Water/water radial distribution function

R	g(OO)	INT(OO)	g(OH)	INT(OH)	g(HH)	INT(HH)
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.15000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.20000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.25000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.30000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.35000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.40000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.45000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.55000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.60000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.65000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.70000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.75000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.80000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.85000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.90000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.95000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.15000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.20000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.25000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.30000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.35000	0.00000	0.00000	0.00002	0.00000	0.00000	0.00000
1.40000	0.00000	0.00000	0.00028	0.00002	0.00000	0.00000
1.45000	0.00000	0.00000	0.00224	0.00017	0.00000	0.00000
1.50000	0.00000	0.00000	0.01185	0.00103	0.00000	0.00000
1.55000	0.00000	0.00000	0.04001	0.00413	0.00000	0.00000
1.60000	0.00000	0.00000	0.10997	0.01319	0.00004	0.00000
1.65000	0.00000	0.00000	0.23422	0.03373	0.00019	0.00002
1.70000	0.00000	0.00000	0.41875	0.07270	0.00077	0.00009
1.75000	0.00000	0.00000	0.63388	0.13521	0.00275	0.00036
1.80000	0.00000	0.00000	0.85348	0.22425	0.00756	0.00115
1.85000	0.00000	0.00000	1.00366	0.33487	0.01812	0.00315

C. Water/water radial distribution function

R	g(OO)	INT(OO)	g(OH)	INT(OH)	g(HH)	INT(HH)
3.80000	0.86937	5.24337	1.09009	10.99607	1.14468	10.13871
3.85000	0.88500	5.45458	1.05107	11.49775	1.14933	10.68730
3.90000	0.89603	5.67401	1.01869	11.99669	1.14553	11.24836
3.95000	0.91051	5.90274	0.99624	12.49723	1.13640	11.81932
4.00000	0.92465	6.14094	0.97830	13.00127	1.11887	12.39578
4.05000	0.93417	6.38765	0.96840	13.51277	1.09878	12.97614
4.10000	0.94064	6.64223	0.96045	14.03266	1.07966	13.56057
4.15000	0.94889	6.90536	0.95362	14.56153	1.05947	14.14814
4.20000	0.95676	7.17709	0.94817	15.10012	1.04276	14.74046
4.25000	0.97077	7.45941	0.94425	15.64934	1.02676	15.33767
4.30000	0.98663	7.75313	0.93881	16.20830	1.01805	15.94382
4.35000	1.00164	8.05830	0.93599	16.77863	1.01352	16.56139
4.40000	1.00902	8.37282	0.93000	17.35840	1.00804	17.18980
4.45000	1.01972	8.69794	0.92613	17.94896	1.00522	17.83080
4.50000	1.02955	9.03362	0.92337	18.55107	1.00406	18.48552
4.55000	1.04203	9.38095	0.92144	19.16534	1.00243	19.15378
4.60000	1.04802	9.73800	0.92338	19.79451	1.00536	19.83881
4.65000	1.05050	10.10372	0.92522	20.43871	1.00766	20.54041
4.70000	1.05735	10.47978	0.92589	21.09731	1.01239	21.26054
4.75000	1.05726	10.86386	0.92839	21.77180	1.01512	21.99806
4.80000	1.06654	11.25950	0.93069	22.46230	1.01887	22.75398
4.85000	1.06851	11.66418	0.93511	23.17059	1.01766	23.52481
4.90000	1.06507	12.07591	0.94175	23.89870	1.01773	24.31168
4.95000	1.06385	12.49560	0.94819	24.64682	1.01717	25.11424
5.00000	1.05350	12.91966	0.95837	25.41833	1.01471	25.93112
5.05000	1.04834	13.35011	0.96747	26.21283	1.01244	26.76254
5.10000	1.03936	13.78537	0.98020	27.03380	1.00979	27.60829
5.15000	1.02841	14.22454	0.99166	27.88074	1.00509	28.46669
5.20000	1.02285	14.66984	1.00303	28.75409	1.00436	29.34120
5.25000	1.01652	15.12095	1.01425	29.65428	0.99945	30.22826
5.30000	1.00824	15.57695	1.02758	30.58376	0.99670	31.12981
5.35000	0.99822	16.03697	1.03921	31.54156	0.99625	32.04803
5.40000	0.99901	16.50600	1.04902	32.52658	0.99808	32.98521
5.45000	0.98995	16.97942	1.05857	33.53906	0.99827	33.94002
5.50000	0.98822	17.46072	1.06576	34.57721	1.00057	34.91466
5.55000	0.98377	17.94861	1.07207	35.64058	1.00269	35.90921
5.60000	0.98656	18.44673	1.07880	36.72998	1.00815	36.92726
5.65000	0.98606	18.95354	1.08350	37.84375	1.01040	37.96590

C. Water/water radial distribution function

R	g(OO)	INT(OO)	g(OH)	INT(OH)	g(HH)	INT(HH)
5.70000	0.98782	19.47028	1.08924	38.98334	1.01671	39.02960
5.75000	0.99108	19.99785	1.09258	40.14656	1.02187	40.11754
5.80000	1.00282	20.54100	1.09277	41.33031	1.02565	41.22858
5.85000	1.00897	21.09694	1.09387	42.53575	1.03256	42.36647
5.90000	1.01916	21.66814	1.08923	43.75670	1.03950	43.53168
5.95000	1.03463	22.25787	1.08642	44.99522	1.04589	44.72400
6.00000	1.04381	22.86288	1.08136	46.24879	1.05166	45.94313
6.05000	1.04884	23.48099	1.07822	47.51964	1.05694	47.18889
6.10000	1.05274	24.11168	1.07385	48.80634	1.06150	48.46078
6.15000	1.05958	24.75693	1.07137	50.11119	1.06221	49.75449
6.20000	1.06571	25.41650	1.06686	51.43176	1.06464	51.07231
6.25000	1.07574	26.09306	1.05973	52.76476	1.06581	52.41296
6.30000	1.08176	26.78433	1.05370	54.11145	1.06423	53.77313
6.35000	1.09080	27.49249	1.04853	55.47290	1.06266	55.15292
6.40000	1.09444	28.21425	1.04333	56.84901	1.06145	56.55293
6.45000	1.09666	28.94882	1.04056	58.24301	1.05698	57.96893
6.50000	1.09634	29.69461	1.03554	59.65187	1.05441	59.40346
6.55000	1.09428	30.45049	1.03094	61.07613	1.05125	60.85577
6.60000	1.09424	31.21793	1.02617	62.51552	1.04756	62.32516
6.65000	1.08444	31.99005	1.02246	63.97153	1.04314	63.81062
6.70000	1.08191	32.77200	1.01905	65.44458	1.03773	65.31067
6.75000	1.07444	33.56020	1.01565	66.93472	1.03307	66.82637
6.80000	1.06275	34.35139	1.01209	68.44171	1.02816	68.35730
6.85000	1.05393	35.14761	1.01099	69.96928	1.02352	69.90379
6.90000	1.04596	35.94939	1.00675	71.51273	1.01877	71.46568
6.95000	1.03796	36.75661	1.00358	73.07370	1.01491	73.04428
7.00000	1.03251	37.57118	0.99984	74.65132	1.01035	74.63847
7.05000	1.02667	38.39276	0.99790	76.24846	1.00776	76.25139
7.10000	1.01685	39.21806	0.99418	77.86227	1.00604	77.88446
7.15000	1.00787	40.04765	0.99486	79.50002	1.00415	79.53751
7.20000	1.00187	40.88387	0.99400	81.15932	1.00129	81.20898
7.25000	0.99534	41.72621	0.99362	82.84109	0.99973	82.90111
7.30000	0.99398	42.57904	0.99382	84.54649	0.99827	84.61415
7.35000	0.98836	43.43871	0.99383	86.27536	0.99838	86.35092
7.40000	0.98443	44.30666	0.99311	88.02657	0.99639	88.10789
7.45000	0.98049	45.18285	0.99327	89.80179	0.99513	89.88644
7.50000	0.97949	46.06993	0.99480	91.60370	0.99386	91.68665
7.55000	0.97582	46.96552	0.99491	93.42992	0.99411	93.51138

C. Water/water radial distribution function

R	g(OO)	INT(OO)	g(OH)	INT(OH)	g(HH)	INT(HH)
7.60000	0.97172	47.86919	0.99445	95.27954	0.99418	95.36052
7.65000	0.96895	48.78218	0.99658	97.15759	0.99334	97.23248
7.70000	0.96552	49.70387	0.99721	99.06148	0.99373	99.12973
7.75000	0.96369	50.63580	0.99887	100.99338	0.99388	101.05199
7.80000	0.96244	51.57858	0.99987	102.95226	0.99343	102.99825
7.85000	0.95802	52.52910	1.00232	104.94119	0.99420	104.97105
7.90000	0.95689	53.49062	1.00289	106.95670	0.99424	106.96916
7.95000	0.95614	54.46358	1.00552	109.00314	0.99525	108.99469
8.00000	0.95895	55.45172	1.00588	111.07614	0.99659	111.04855
8.05000	0.96462	56.45816	1.00821	113.17999	0.99836	113.13187
8.10000	0.97031	57.48315	1.01128	115.31656	0.99915	115.24281
8.15000	0.97588	58.52681	1.01119	117.47939	1.00073	117.38327
8.20000	0.98113	59.58899	1.01447	119.67593	1.00068	119.54996
8.25000	0.98528	60.66870	1.01434	121.89908	0.99976	121.74115
8.30000	0.98996	61.76674	1.01312	124.14653	0.99771	123.95441
8.35000	0.99209	62.88043	1.01210	126.41885	0.99632	126.19130
8.40000	1.00018	64.01669	1.01032	128.71443	0.99436	128.45061
8.45000	1.00668	65.17400	1.00990	131.03645	0.99272	130.73314
8.50000	1.01080	66.34982	1.00710	133.37952	0.99075	133.03816
8.55000	1.01619	67.54587	1.00561	135.74673	0.98747	135.36266
8.60000	1.01869	68.75893	1.00328	138.13617	0.98484	137.70816
8.65000	1.02536	69.99417	1.00159	140.54939	0.98018	140.06979
8.70000	1.02907	71.24825	0.99807	142.98199	0.97712	142.45135
8.75000	1.03492	72.52400	0.99349	145.43137	0.97218	144.84818
8.80000	1.03771	73.81786	0.99013	147.90044	0.97546	147.25571
8.85000	1.04045	75.12991	0.98572	150.38652	0.97621	149.67491
8.90000	1.04263	76.45963	0.98027	152.88686	0.97857	152.10716
8.95000	1.04362	77.80559	0.98450	155.40050	0.97689	154.54959
9.00000	1.04380	66.34982	1.00710	133.37952	0.97075	133.03816
9.05000	1.04319	67.54587	1.00561	135.74673	0.97747	135.36266
9.10000	1.04369	68.75893	1.00328	138.13617	0.98484	137.70816
9.15000	1.04336	69.99417	1.00159	140.54939	0.98018	140.06979
9.20000	1.04307	71.24825	1.00807	142.98199	0.98712	142.45135
9.25000	1.04392	72.52400	1.00349	145.43137	0.98218	144.84818
9.30000	1.04371	73.81786	1.00013	147.90044	0.98546	147.25571
9.35000	1.04345	75.12991	1.00572	150.38652	0.98921	149.67491
9.40000	1.04363	76.45963	1.00027	152.88686	0.98357	152.10716
9.45000	1.04362	77.80559	1.00450	155.40050	0.98689	154.54959

C. Water/water radial distribution function

R	g(OO)	INT(OO)	g(OH)	INT(OH)	g(HH)	INT(HH)
9.50000	1.04319	67.54587	1.00561	135.74673	0.98747	135.36266
9.55000	1.04369	68.75893	1.00328	138.13617	0.98484	137.70816
9.60000	1.04336	69.99417	1.00259	140.54939	0.98018	140.06979
9.65000	1.04307	71.24825	1.00307	142.98199	0.98712	142.45135
9.70000	1.04392	72.52400	1.00349	145.43137	0.98218	144.84818
9.75000	1.04371	73.81786	1.00013	147.90044	0.98546	147.25571
9.80000	1.04345	75.12991	1.00272	150.38652	0.98921	149.67491
9.85000	1.04363	76.45963	1.00027	152.88686	0.98357	152.10716
9.90000	1.04362	77.80559	1.00150	155.40050	0.98689	154.54959
9.95000	1.04263	76.45963	1.00027	152.88686	0.98357	152.10716
10.00000	1.04362	77.80559	1.00150	155.40050	0.98689	154.54959

D. Ammonia/water radial distribution function

R	g(NO)	INT(NO)	g(NH)	INT(NH)	g(OH)	INT(OH)
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.15000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.20000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.25000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.30000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.35000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.40000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.45000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.55000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.60000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.65000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.70000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.75000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.80000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.85000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.90000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.95000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

D. Ammonia/water radial distribution function

R	g(NO)	INT(NO)	g(NH)	INT(NH)	g(OH)	INT(OH)
1.15000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.20000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.25000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.30000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.35000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.40000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.45000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.50000	0.00000	0.00000	0.00022	0.00002	0.00000	0.00000
1.55000	0.00000	0.00000	0.00151	0.00013	0.00002	0.00000
1.60000	0.00000	0.00000	0.00735	0.00074	0.00013	0.00002
1.65000	0.00000	0.00000	0.02686	0.00309	0.00137	0.00020
1.70000	0.00000	0.00000	0.06897	0.00951	0.00533	0.00094
1.75000	0.00000	0.00000	0.16055	0.02535	0.01768	0.00356
1.80000	0.00000	0.00000	0.30277	0.05693	0.04309	0.01030
1.85000	0.00000	0.00000	0.47442	0.10922	0.09081	0.02531
1.90000	0.00000	0.00000	0.63972	0.18359	0.16249	0.05365
1.95000	0.00000	0.00000	0.76998	0.27787	0.25939	0.10129
2.00000	0.00000	0.00000	0.83730	0.38572	0.37090	0.17295
2.05000	0.00000	0.00000	0.83270	0.49840	0.48845	0.27210
2.10000	0.00000	0.00000	0.77093	0.60788	0.59065	0.39792
2.15000	0.00000	0.00000	0.69749	0.71170	0.67249	0.54807
2.20000	0.00000	0.00000	0.61458	0.80749	0.73459	0.71980
2.25000	0.00000	0.00000	0.54694	0.89665	0.76774	0.90754
2.30000	0.00000	0.00000	0.49104	0.98030	0.78695	1.10862
2.35000	0.00000	0.00000	0.45772	1.06169	0.79310	1.32018
2.40000	0.00014	0.00001	0.42640	1.14078	0.78593	1.53884
2.45000	0.00083	0.00009	0.42467	1.22287	0.78975	1.76781
2.50000	0.00444	0.00054	0.43127	1.30966	0.79976	2.00925
2.55000	0.02120	0.00276	0.45949	1.40587	0.82366	2.26795
2.60000	0.06085	0.00938	0.50853	1.51657	0.85966	2.54864
2.65000	0.15313	0.02670	0.57012	1.64549	0.89091	2.85084
2.70000	0.32370	0.06469	0.65695	1.79971	0.94259	3.18275
2.75000	0.57200	0.13434	0.76175	1.98522	1.00390	3.54946
2.80000	0.89206	0.24694	0.87234	2.20545	1.07069	3.95492
2.85000	1.25450	0.41100	1.00497	2.46831	1.15354	4.40749
2.90000	1.61587	0.62980	1.15081	2.77996	1.23307	4.90839
2.95000	1.94407	0.90220	1.29709	3.14345	1.31364	5.46057
3.00000	2.21871	1.22371	1.44362	3.56183	1.40145	6.06981

D. Ammonia/water radial distribution function

R	g(NO)	INT(NO)	g(NH)	INT(NH)	g(OH)	INT(OH)
3.05000	2.43314	1.58813	1.58166	4.03562	1.48289	6.73612
3.10000	2.59060	1.98897	1.71472	4.56625	1.55523	7.45803
3.15000	2.69400	2.41936	1.82020	5.14784	1.62251	8.23567
3.20000	2.71942	2.86772	1.90825	5.77708	1.68206	9.06764
3.25000	2.71690	3.32977	1.95675	6.44262	1.71964	9.94499
3.30000	2.65403	3.79511	1.97281	7.13443	1.75405	10.86763
3.35000	2.53806	4.25372	1.94490	7.83728	1.75994	11.82165
3.40000	2.41221	4.70269	1.89976	8.54446	1.76016	12.80448
3.45000	2.28178	5.13997	1.84157	9.25029	1.74309	13.80661
3.50000	2.14807	5.56364	1.77070	9.94878	1.71772	14.82299
3.55000	2.01034	5.97156	1.69202	10.63543	1.67512	15.84268
3.60000	1.87824	6.36348	1.61875	11.31099	1.61974	16.85663
3.65000	1.74785	6.73840	1.54263	11.97278	1.56003	17.86050
3.70000	1.62322	7.09619	1.47784	12.62427	1.49357	18.84813
3.75000	1.50199	7.43626	1.40598	13.26095	1.43605	19.82356
3.80000	1.41592	7.76545	1.35025	13.88880	1.37596	20.78326
3.85000	1.31953	8.08036	1.30192	14.51021	1.31857	21.72729
3.90000	1.23739	8.38339	1.26054	15.12760	1.26334	22.65544
3.95000	1.16852	8.67693	1.22417	15.74265	1.21460	23.57080
4.00000	1.11660	8.96458	1.20163	16.36176	1.16516	24.47127
4.05000	1.04690	9.24106	1.17146	16.98050	1.13420	25.36986
4.10000	0.98660	9.50809	1.14683	17.60127	1.09936	26.26248
4.15000	0.94034	9.76884	1.12226	18.22366	1.06538	27.14874
4.20000	0.90673	10.02637	1.08601	18.84055	1.03668	28.03204
4.25000	0.86911	10.27912	1.05968	19.45689	1.00712	28.91071
4.30000	0.83907	10.52891	1.02462	20.06696	0.97763	29.78383
4.35000	0.81091	10.77597	0.99022	20.67032	0.94549	30.64799
4.40000	0.78435	11.02046	0.95898	21.26816	0.91616	31.50471
4.45000	0.76910	11.26567	0.92388	21.85728	0.89008	32.35608
4.50000	0.74590	11.50887	0.89686	22.44209	0.86835	33.20543
4.55000	0.73325	11.75328	0.87530	23.02560	0.84845	34.05385
4.60000	0.72562	12.00049	0.84725	23.60291	0.83434	34.90660
4.65000	0.71677	12.25003	0.83024	24.18097	0.82141	35.76448
4.70000	0.70057	12.50133	0.82095	24.76492	0.81631	36.63548
4.75000	0.70548	12.75761	0.80494	25.34975	0.80762	37.51563
4.80000	0.70129	13.01739	0.79775	25.94160	0.80032	38.40628
4.85000	0.70197	13.28324	0.79237	26.54178	0.79390	39.30829
4.90000	0.70195	13.55460	0.78448	27.14830	0.79236	40.22722

D. Ammonia/water radial distribution function

R	g(NO)	INT(NO)	g(NH)	INT(NH)	g(OH)	INT(OH)
6.85000	1.05363	34.78038	1.04990	69.05519	1.02028	103.76462
6.90000	1.04880	35.58434	1.04933	70.66393	1.02535	106.12257
6.95000	1.04605	36.39786	1.04818	72.29428	1.02489	108.51375
7.00000	1.04120	37.21928	1.04657	73.94562	1.02780	110.94635
7.05000	1.03597	38.04831	1.04428	75.61697	1.03025	113.41969
7.10000	1.03566	38.88889	1.04616	77.31517	1.03471	115.93912
7.15000	1.02898	39.73584	1.04716	79.03902	1.03607	118.49751
7.20000	1.02422	40.59071	1.04542	80.78416	1.03849	121.09787
7.25000	1.01899	41.45306	1.04673	82.55585	1.03859	123.73473
7.30000	1.01319	42.32237	1.04619	84.35112	1.04021	126.41223
7.35000	1.00934	43.20029	1.04329	86.16603	1.03941	129.12447
7.40000	1.00103	44.08287	1.04155	88.00264	1.03739	131.86838
7.45000	1.00244	44.97868	1.04149	89.86404	1.03499	134.64307
7.50000	1.00339	45.88742	1.03875	91.74556	1.03181	137.44647
7.55000	1.00453	46.80936	1.03399	93.64351	1.02863	140.27864
7.60000	1.00734	47.74615	1.02970	95.55870	1.02792	143.14645
7.65000	1.00609	48.69414	1.02437	97.48914	1.02686	146.04915
7.70000	1.01111	49.65935	1.02166	99.43971	1.02327	148.97963
7.75000	1.01164	50.63765	1.01909	101.41074	1.02722	151.95975
7.80000	1.01670	51.63356	1.01698	103.40314	1.02815	154.98117
7.85000	1.01934	52.64491	1.01539	105.41801	1.02607	158.03528
7.90000	1.01914	53.66899	1.00959	107.44698	1.02708	161.13144
7.95000	1.02360	54.71060	1.00503	109.49242	1.02556	164.26228
8.00000	1.02587	55.76770	1.00299	111.55946	1.02569	167.43303
8.05000	1.02374	56.83583	1.00187	113.65010	1.02653	170.64616
8.10000	1.02071	57.91406	1.00251	115.76814	1.02389	173.89096
8.15000	1.02262	59.00769	1.00211	117.91156	1.02229	177.17084
8.20000	1.02222	60.11435	1.00297	120.08322	1.01946	180.48187
8.25000	1.02373	61.23621	1.00472	122.28526	1.01846	183.83014
8.30000	1.02231	62.37013	1.00559	124.51602	1.01351	187.20262
8.35000	1.01847	63.51344	1.00524	126.77295	1.01144	190.60890
8.40000	1.01588	64.66754	1.00763	129.06241	1.00884	194.04724
8.45000	1.01548	65.83496	1.00771	131.37941	1.00582	197.51620
8.50000	1.01607	67.01692	1.00751	133.72342	1.00304	201.01665
8.55000	1.01307	68.20930	1.00739	136.09482	1.00085	204.55066
8.60000	1.01300	69.41559	1.00317	138.48396	0.99551	208.10706
8.65000	1.00798	70.62988	1.00323	140.90112	0.99278	211.69504
8.70000	1.00954	71.86017	0.99896	143.33591	0.98893	215.31056

D. Ammonia/water radial distribution function

R	g(NO)	INT(NO)	g(NH)	INT(NH)	g(OH)	INT(OH)
4.95000	0.70723	13.83361	0.78213	27.76541	0.79258	41.16525
5.00000	0.71566	14.12167	0.78494	28.39731	0.80216	42.13390
5.05000	0.71960	14.41715	0.78741	29.04393	0.81266	43.13495
5.10000	0.72252	14.71972	0.79527	29.71001	0.82337	44.16937
5.15000	0.73192	15.03228	0.80497	30.39749	0.83373	45.23746
5.20000	0.74069	15.35474	0.80848	31.10146	0.84844	46.34558
5.25000	0.74743	15.68643	0.81802	31.82748	0.86092	47.49174
5.30000	0.75237	16.02670	0.82516	32.57387	0.87769	48.68259
5.35000	0.76312	16.37837	0.83235	33.34102	0.89030	49.91345
5.40000	0.78139	16.74522	0.84145	34.13113	0.90164	51.18340
5.45000	0.79192	17.12393	0.84898	34.94315	0.91120	52.49069
5.50000	0.80668	17.51682	0.86192	35.78273	0.91954	53.83426
5.55000	0.82114	17.92404	0.86935	36.64502	0.93267	55.22189
5.60000	0.84571	18.35104	0.87768	37.53133	0.94068	56.64679
5.65000	0.86095	18.79355	0.88722	38.44333	0.94972	58.11118
5.70000	0.88609	19.25706	0.89901	39.38390	0.95670	59.61255
5.75000	0.90308	19.73779	0.90531	40.34773	0.96525	61.15404
5.80000	0.92645	20.23958	0.91739	41.34149	0.97009	62.73032
5.85000	0.95504	20.76581	0.92858	42.36479	0.97779	64.34662
5.90000	0.98108	21.31566	0.93745	43.41560	0.98132	65.99660
5.95000	1.00234	21.88699	0.95270	44.50169	0.98275	67.67711
6.00000	1.02054	22.47852	0.95942	45.61391	0.99064	69.39970
6.05000	1.03730	23.08981	0.97040	46.75766	0.99042	71.15074
6.10000	1.04966	23.71867	0.97881	47.93047	0.99258	72.93472
6.15000	1.06004	24.36420	0.98490	49.13000	0.99598	74.75429
6.20000	1.05980	25.02011	0.99750	50.36473	0.99585	76.60332
6.25000	1.07401	25.69559	1.00609	51.63025	0.99511	78.48090
6.30000	1.08183	26.38692	1.01611	52.92889	0.99772	80.39363
6.35000	1.09085	27.09511	1.02713	54.26256	0.99669	82.33484
6.40000	1.09717	27.81866	1.03659	55.62978	1.00019	84.31366
6.45000	1.10152	28.55649	1.04046	57.02364	1.00392	86.33102
6.50000	1.10382	29.30736	1.04320	58.44292	1.00596	88.38394
6.55000	1.10368	30.06973	1.04608	59.88809	1.00910	90.47507
6.60000	1.09860	30.84023	1.04758	61.35753	1.00969	92.59949
6.65000	1.09597	31.62056	1.04938	62.85187	1.01054	94.75803
6.70000	1.08552	32.40512	1.04664	64.36479	1.01192	96.95215
6.75000	1.07296	33.19223	1.04807	65.90250	1.01479	99.18547
6.80000	1.06403	33.98439	1.05194	67.46883	1.01488	101.45219

D. Ammonia/water radial distribution function

R	g(NO)	INT(NO)	g(NH)	INT(NH)	g(OH)	INT(OH)
8.75000	1.00792	73.10265	0.99594	145.79132	0.98510	218.95358
8.80000	1.00546	74.35629	0.99005	148.26018	0.98092	222.62273
8.85000	1.00804	75.62747	0.98472	150.74373	0.97550	226.31317
8.90000	1.01370	76.92029	0.98170	153.24771	0.96800	230.01674
8.95000	1.01886	78.23431	0.97615	155.76559	0.96259	233.74110
9.00000	1.02587	55.76770	1.00299	111.55946	1.02569	167.43303
9.05000	1.02374	56.83583	1.00187	113.65010	1.02653	170.64616
9.10000	1.02071	57.91406	1.00251	115.76814	1.02389	173.89096
9.15000	1.02262	59.00769	1.00211	117.91156	1.02229	177.17084
9.20000	1.02222	60.11435	1.00297	120.08322	1.01946	180.48187
9.25000	1.02373	61.23621	1.00472	122.28526	1.01846	183.83014
9.30000	1.02231	62.37013	1.00559	124.51602	1.01351	187.20262
9.35000	1.01847	63.51344	1.00524	126.77295	1.01144	190.60890
9.40000	1.01588	64.66754	1.00763	129.06241	1.00884	194.04724
9.45000	1.01548	65.83496	1.00771	131.37941	1.00582	197.51620
9.50000	1.01607	67.01692	1.00751	133.72342	1.00304	201.01665
9.55000	1.01307	68.20930	1.00739	136.09482	1.00085	204.55066
9.60000	1.01300	69.41559	1.00317	138.48396	0.99551	208.10706
9.65000	1.00798	70.62988	1.00323	140.90112	0.99278	211.69504
9.70000	1.00954	71.86017	0.99896	143.33591	0.98893	215.31056
9.75000	1.00792	73.10265	0.99594	145.79132	0.98510	218.95358
9.80000	1.00546	74.35629	0.99005	148.26018	0.98092	222.62273
9.85000	1.00804	75.62747	0.98472	150.74373	0.97550	226.31317
9.90000	1.01370	76.92029	0.98170	153.24771	0.96800	230.01674
9.95000	1.01886	78.23431	0.97615	155.76559	0.96259	233.74110
10.00000	1.02587	55.76770	1.00299	111.55946	1.02569	167.43303

E. Water/ammonia radial distribution function

R	g(ON)	INT(ON)	g(OH)	INT(OH)	g(NH)	INT(NH)
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.15000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.20000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.25000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.30000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.35000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000

E. Water/ammonia radial distribution function

R	g(CN)	INT(ON)	g(OH)	INT(OH)	g(NH)	INT(NH)
0.40000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.45000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.55000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.60000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.65000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.70000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.75000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.80000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.85000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.90000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.95000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.15000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.20000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.25000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.30000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.35000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.40000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.45000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.50000	0.00000	0.00000	0.00000	0.00000	0.00022	0.00000
1.55000	0.00000	0.00000	0.00002	0.00000	0.00151	0.00003
1.60000	0.00000	0.00000	0.00013	0.00000	0.00735	0.00017
1.65000	0.00000	0.00000	0.00137	0.00005	0.02686	0.00072
1.70000	0.00000	0.00000	0.00533	0.00022	0.06897	0.00222
1.75000	0.00000	0.00000	0.01768	0.00083	0.16055	0.00591
1.80000	0.00000	0.00000	0.04309	0.00240	0.30277	0.01327
1.85000	0.00000	0.00000	0.09081	0.00590	0.47442	0.02546
1.90000	0.00000	0.00000	0.16249	0.01251	0.63972	0.04280
1.95000	0.00000	0.00000	0.25939	0.02361	0.76998	0.06478
2.00000	0.00000	0.00000	0.37090	0.04032	0.83730	0.08992
2.05000	0.00000	0.00000	0.48845	0.06343	0.83270	0.11619
2.10000	0.00000	0.00000	0.59065	0.09277	0.77093	0.14171
2.15000	0.00000	0.00000	0.67249	0.12777	0.69749	0.16592
2.20000	0.00000	0.00000	0.73459	0.16781	0.61458	0.18825
2.25000	0.00000	0.00000	0.76774	0.21157	0.54694	0.20903

E. Water/ammonia radial distribution function

R	g(ON)	INT(ON)	g(OH)	INT(OH)	g(NH)	INT(NH)
2.30000	0.00000	0.00000	0.78695	0.25845	0.49104	0.22854
2.35000	0.00000	0.00000	0.79310	0.30777	0.45772	0.24751
2.40000	0.00014	0.00000	0.78593	0.35875	0.42640	0.26595
2.45000	0.00083	0.00002	0.78975	0.41213	0.42467	0.28509
2.50000	0.00444	0.00013	0.79976	0.46841	0.43127	0.30532
2.55000	0.02120	0.00064	0.82366	0.52872	0.45949	0.32775
2.60000	0.06085	0.00219	0.85966	0.59416	0.50853	0.35356
2.65000	0.15313	0.00622	0.89091	0.66461	0.57012	0.38361
2.70000	0.32370	0.01508	0.94259	0.74199	0.65695	0.41957
2.75000	0.57200	0.03132	1.00390	0.82748	0.76175	0.46281
2.80000	0.89206	0.05757	1.07069	0.92201	0.87234	0.51415
2.85000	1.25450	0.09582	1.15354	1.02751	1.00497	0.57543
2.90000	1.61587	0.14683	1.23307	1.14429	1.15081	0.64809
2.95000	1.94407	0.21033	1.31364	1.27302	1.29709	0.73283
3.00000	2.21871	0.28528	1.40145	1.41505	1.44362	0.83037
3.05000	2.43314	0.37024	1.48289	1.57038	1.58166	0.94082
3.10000	2.59060	0.46369	1.55523	1.73868	1.71472	1.06453
3.15000	2.69400	0.56402	1.62251	1.91997	1.82020	1.20011
3.20000	2.71942	0.66855	1.68206	2.11392	1.90825	1.34680
3.25000	2.71690	0.77626	1.71964	2.31846	1.95675	1.50196
3.30000	2.65403	0.88475	1.75405	2.53356	1.97281	1.66324
3.35000	2.53806	0.99166	1.75994	2.75596	1.94490	1.82709
3.40000	2.41221	1.09633	1.76016	2.98509	1.89976	1.99196
3.45000	2.28178	1.19827	1.74309	3.21871	1.84157	2.15651
3.50000	2.14807	1.29704	1.71772	3.45566	1.77070	2.31935
3.55000	2.01034	1.39214	1.67512	3.69338	1.69202	2.47942
3.60000	1.87824	1.48351	1.61974	3.92976	1.61875	2.63691
3.65000	1.74785	1.57091	1.56003	4.16380	1.54263	2.79120
3.70000	1.62322	1.65432	1.49357	4.39404	1.47784	2.94308
3.75000	1.50199	1.73360	1.43605	4.62144	1.40598	3.09151
3.80000	1.41592	1.81035	1.37596	4.84518	1.35025	3.23787
3.85000	1.31953	1.88376	1.31857	5.06526	1.30192	3.38274
3.90000	1.23739	1.95441	1.26334	5.28164	1.26054	3.52667
3.95000	1.16852	2.02284	1.21460	5.49504	1.22417	3.67006
4.00000	1.11660	2.08990	1.16516	5.70496	1.20163	3.81439
4.05000	1.04690	2.15435	1.13420	5.91445	1.17146	3.95864
4.10000	0.98660	2.21661	1.09936	6.12255	1.14683	4.10336
4.15000	0.94034	2.27739	1.06538	6.32917	1.12226	4.24846

E. Water/ammonia radial distribution function

R	g(ON)	INT(ON)	g(OH)	INT(OH)	g(NH)	INT(NH)
4.20000	0.90673	2.33743	1.03668	6.53509	1.08601	4.39228
4.25000	0.86911	2.39635	1.00712	6.73993	1.05968	4.53597
4.30000	0.83907	2.45459	0.97763	6.94348	1.02462	4.67819
4.35000	0.81091	2.51218	0.94549	7.14495	0.99022	4.81885
4.40000	0.78435	2.56918	0.91616	7.34468	0.95898	4.95823
4.45000	0.76910	2.62635	0.89008	7.54315	0.92388	5.09557
4.50000	0.74590	2.68304	0.86835	7.74116	0.89686	5.23191
4.55000	0.73325	2.74002	0.84845	7.93895	0.87530	5.36794
4.60000	0.72562	2.79765	0.83434	8.13776	0.84725	5.50253
4.65000	0.71677	2.85583	0.82141	8.33776	0.83024	5.63729
4.70000	0.70657	2.91441	0.81631	8.54081	0.82095	5.77343
4.75000	0.70548	2.97416	0.80762	8.74600	0.80494	5.90977
4.80000	0.70029	3.03472	0.80032	8.95364	0.79775	6.04775
4.85000	0.70197	3.09670	0.79390	9.16392	0.79237	6.18767
4.90000	0.70195	3.15996	0.79236	9.37815	0.78448	6.32907
4.95000	0.70723	3.22500	0.79258	9.59683	0.78213	6.47294
5.00000	0.71566	3.29216	0.80216	9.82265	0.78494	6.62025
5.05000	0.71960	3.36104	0.81266	10.05603	0.78741	6.77100
5.10000	0.72252	3.43158	0.82337	10.29718	0.79527	6.92629
5.15000	0.73192	3.50445	0.83373	10.54619	0.80497	7.08656
5.20000	0.74069	3.57962	0.84844	10.80452	0.80848	7.25068
5.25000	0.74743	3.65695	0.86092	11.07173	0.81802	7.41994
5.30000	0.75237	3.73628	0.87769	11.34935	0.82516	7.59394
5.35000	0.76312	3.81826	0.89030	11.63630	0.83235	7.77279
5.40000	0.78139	3.90379	0.90164	11.93236	0.84145	7.95699
5.45000	0.79192	3.99208	0.91120	12.23713	0.84898	8.14629
5.50000	0.80668	4.08367	0.91954	12.55036	0.86192	8.34203
5.55000	0.82114	4.17861	0.93267	12.87386	0.86935	8.54305
5.60000	0.84571	4.27816	0.94068	13.20605	0.87768	8.74968
5.65000	0.86095	4.38132	0.94972	13.54744	0.88722	8.96229
5.70000	0.88609	4.48938	0.95670	13.89745	0.89901	9.18157
5.75000	0.90308	4.60146	0.96525	14.25682	0.90531	9.40627
5.80000	0.92645	4.71844	0.97009	14.62430	0.91739	9.63794
5.85000	0.95504	4.84112	0.97779	15.00110	0.92858	9.87651
5.90000	0.98108	4.96931	0.98132	15.38577	0.93745	10.12148
5.95000	1.00234	5.10250	0.98275	15.77754	0.95270	10.37468
6.00000	1.02054	5.24040	0.99064	16.17912	0.95942	10.63397
6.05000	1.03730	5.38292	0.99042	16.58734	0.97040	10.90061

E. Water/ammonia radial distribution function

R	g(ON)	INT(ON)	g(OH)	INT(OH)	g(NH)	INT(NH)
6.10000	1.04966	5.52952	0.99258	17.00323	0.97881	11.17403
6.15000	1.06004	5.68002	0.99598	17.42743	0.98490	11.45368
6.20000	1.05980	5.83293	0.99585	17.85849	0.99750	11.74153
6.25000	1.07401	5.99040	0.99511	18.29620	1.00609	12.03656
6.30000	1.08183	6.15157	0.99772	18.74211	1.01611	12.33932
6.35000	1.09085	6.31657	0.99669	19.19466	1.02713	12.65023
6.40000	1.09717	6.48536	1.00019	19.65598	1.03659	12.96897
6.45000	1.10152	6.65737	1.00392	20.12628	1.04046	13.29392
6.50000	1.10382	6.83242	1.00596	20.60487	1.04320	13.62480
6.55000	1.10368	7.01015	1.00910	21.09238	1.04608	13.96171
6.60000	1.09860	7.18978	1.00969	21.58763	1.04758	14.30428
6.65000	1.09597	7.37170	1.01054	22.09085	1.04938	14.65266
6.70000	1.08552	7.55460	1.01192	22.60236	1.04664	15.00537
6.75000	1.07296	7.73810	1.01479	23.12300	1.04807	15.36385
6.80000	1.06403	7.92278	1.01488	23.65143	1.05194	15.72901
6.85000	1.05363	8.10835	1.02028	24.19052	1.04990	16.09883
6.90000	1.04880	8.29578	1.02535	24.74022	1.04933	16.47386
6.95000	1.04605	8.48543	1.02489	25.29767	1.04818	16.85394
7.00000	1.04120	8.67693	1.02780	25.86478	1.04657	17.23891
7.05000	1.03597	8.87020	1.03025	26.44138	1.04428	17.62854
7.10000	1.03566	9.06617	1.03471	27.02872	1.04616	18.02443
7.15000	1.02898	9.26362	1.03607	27.62515	1.04716	18.42630
7.20000	1.02422	9.46291	1.03849	28.23137	1.04542	18.83313
7.25000	1.01899	9.66395	1.03859	28.84608	1.04673	19.24615
7.30000	1.01319	9.86662	1.04021	29.47029	1.04619	19.66467
7.35000	1.00934	10.07129	1.03941	30.10258	1.04329	20.08777
7.40000	1.00103	10.27704	1.03739	30.74226	1.04155	20.51593
7.45000	1.00244	10.48588	1.03499	31.38911	1.04149	20.94987
7.50000	1.00339	10.69774	1.03181	32.04266	1.03875	21.38850
7.55000	1.00453	10.91267	1.02863	32.70291	1.03399	21.83096
7.60000	1.00734	11.13106	1.02792	33.37148	1.02970	22.27745
7.65000	1.00609	11.35207	1.02686	34.04817	1.02437	22.72748
7.70000	1.01111	11.57709	1.02327	34.73134	1.02166	23.18221
7.75000	1.01164	11.80516	1.02722	35.42609	1.01909	23.64171
7.80000	1.01670	12.03734	1.02815	36.13046	1.01698	24.10619
7.85000	1.01934	12.27311	1.02607	36.84245	1.01539	24.57591
7.90000	1.01914	12.51185	1.02708	37.56425	1.00959	25.04892
7.95000	1.02360	12.75469	1.02556	38.29414	1.00503	25.52576

E. Water/ammonia radial distribution function

R	g(CN)	INT(ON)	g(OH)	INT(OH)	g(NH)	INT(NH)
8.00000	1.02587	13.00113	1.02569	39.03333	1.00299	26.00764
8.05000	1.02374	13.25014	1.02653	39.78239	1.00187	26.49503
8.10000	1.02071	13.50151	1.02389	40.53885	1.00251	26.98880
8.15000	1.02262	13.75647	1.02229	41.30348	1.00211	27.48848
8.20000	1.02222	14.01446	1.01946	42.07538	1.00297	27.99475
8.25000	1.02373	14.27600	1.01846	42.85594	1.00472	28.50810
8.30000	1.02231	14.54035	1.01351	43.64217	1.00559	29.02815
8.35000	1.01847	14.80689	1.01144	44.43626	1.00524	29.55431
8.40000	1.01588	15.07595	1.00884	45.23784	1.00763	30.08804
8.45000	1.01548	15.34811	1.00582	46.04654	1.00771	30.62819
8.50000	1.01607	15.62366	1.00304	46.86259	1.00751	31.17464
8.55000	1.01307	15.90164	1.00085	47.68646	1.00739	31.72748
8.60000	1.01300	16.18286	0.99551	48.51555	1.00317	32.28445
8.65000	1.00798	16.46594	0.99278	49.35201	1.00323	32.84796
8.70000	1.00954	16.75275	0.98893	50.19489	0.99896	33.41557
8.75000	1.00792	17.04240	0.98510	51.04417	0.99594	33.98799
8.80000	1.00546	17.33466	0.98092	51.89955	0.99005	34.56355
8.85000	1.00804	17.63100	0.97550	52.75990	0.98472	35.14253
8.90000	1.01370	17.93239	0.96800	53.62331	0.98170	35.72627
8.95000	1.01886	18.23872	0.96259	54.49156	0.97615	36.31326
9.00000	1.02587	18.51113	0.98569	39.03333	1.00299	26.00764
9.05000	1.02374	18.25014	1.00653	39.78239	1.00187	26.49503
9.10000	1.02071	18.53151	1.00389	40.53885	1.00251	26.98880
9.15000	1.02262	18.71647	1.00229	41.30348	1.00211	27.48848
9.20000	1.02222	18.98446	1.01946	42.07538	1.00297	27.99475
9.25000	1.02373	19.17600	1.01846	42.85594	1.00472	28.50810
9.30000	1.02231	19.34035	1.01351	43.64217	1.00559	29.02815
9.35000	1.01847	19.59689	1.01144	44.43626	1.00524	29.55431
9.40000	1.01588	19.87595	1.02884	45.23784	1.00763	30.08804
9.45000	1.01548	20.15811	1.02582	46.04654	1.00771	30.62819
9.50000	1.01607	20.43366	1.01304	46.86259	1.00751	31.17464
9.55000	1.01307	20.72164	1.00085	47.68646	1.00739	31.72748
9.60000	1.01300	20.95286	1.01551	48.51555	1.00317	32.28445
9.65000	1.00798	21.23594	1.02278	49.35201	1.00323	32.84796
9.70000	1.00954	21.51275	1.01893	50.19489	0.99896	33.41557
9.75000	1.00792	21.79240	1.01510	51.04417	0.99594	33.98799
9.80000	1.00546	21.98466	1.00092	51.89955	0.99005	34.56355
9.85000	1.00804	22.26100	1.01550	52.75990	0.98472	35.14253

E. Water/ammonia radial distribution function

R	g(ON)	INT(ON)	g(OH)	INT(OH)	g(NH)	INT(NH)
9.90000	1.01370	22.54239	1.01800	53.62331	0.98170	35.72627
9.95000	1.01886	22.82872	1.02259	54.49156	0.97615	36.31326
10.00000	1.01987	23.08113	1.02569	39.03333	1.00299	26.00764

F. Ammonia/ammonia radial distribution function

R	g(NN)	INT(NN)	g(NH)	INT(NH)	g(HH)	INT(HH)
0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.15000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.20000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.25000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.30000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.35000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.40000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.45000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.50000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.55000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.60000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.65000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.70000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.75000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.80000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.85000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.90000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
0.95000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.05000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.10000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.15000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.20000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.25000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.30000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
1.35000	0.00000	0.00000	0.00000	0.00000	0.00017	0.00000
1.40000	0.00000	0.00000	0.00000	0.00000	0.00016	0.00001
1.45000	0.00000	0.00000	0.00000	0.00000	0.00037	0.00002
1.50000	0.00000	0.00000	0.00000	0.00000	0.00084	0.00004

F. Ammonia/ammonia radial distribution function

R	g(NN)	INT(NN)	g(NH)	INT(NH)	g(HH)	INT(HH)
1.55000	0.00000	0.00000	0.00000	0.00000	0.00183	0.00009
1.60000	0.00000	0.00000	0.00000	0.00000	0.00258	0.00016
1.65000	0.00000	0.00000	0.00000	0.00000	0.00428	0.00029
1.70000	0.00000	0.00000	0.00000	0.00000	0.00947	0.00060
1.75000	0.00000	0.00000	0.00000	0.00000	0.01588	0.00115
1.80000	0.00000	0.00000	0.00015	0.00001	0.02734	0.00215
1.85000	0.00000	0.00000	0.00021	0.00001	0.04143	0.00374
1.90000	0.00000	0.00000	0.00078	0.00005	0.05392	0.00593
1.95000	0.00000	0.00000	0.00137	0.00010	0.07726	0.00924
2.00000	0.00000	0.00000	0.00307	0.00024	0.09323	0.01344
2.05000	0.00000	0.00000	0.00652	0.00055	0.11656	0.01896
2.10000	0.00000	0.00000	0.00953	0.00102	0.14062	0.02594
2.15000	0.00000	0.00000	0.01195	0.00165	0.15775	0.03415
2.20000	0.00000	0.00000	0.01804	0.00263	0.17647	0.04377
2.25000	0.00000	0.00000	0.02364	0.00398	0.19523	0.05490
2.30000	0.00000	0.00000	0.04034	0.00638	0.20938	0.06737
2.35000	0.00000	0.00000	0.05120	0.00956	0.23077	0.08172
2.40000	0.00000	0.00000	0.06880	0.01403	0.24423	0.09756
2.45000	0.00000	0.00000	0.08698	0.01990	0.26147	0.11524
2.50000	0.00000	0.00000	0.11239	0.02781	0.26748	0.13406
2.55000	0.00000	0.00000	0.13431	0.03765	0.28359	0.15483
2.60000	0.00000	0.00000	0.15576	0.04951	0.29455	0.17725
2.65000	0.00060	0.00002	0.18379	0.06404	0.31142	0.20188
2.70000	0.00136	0.00005	0.21311	0.08153	0.32533	0.22858
2.75000	0.00431	0.00018	0.24738	0.10260	0.34343	0.25783
2.80000	0.01337	0.00057	0.28956	0.12816	0.35397	0.28908
2.85000	0.02947	0.00147	0.31916	0.15736	0.36510	0.32247
2.90000	0.05776	0.00329	0.34886	0.19039	0.37380	0.35787
2.95000	0.09178	0.00629	0.37337	0.22698	0.38747	0.39584
3.00000	0.13186	0.01074	0.40147	0.26767	0.39599	0.43597
3.05000	0.18999	0.01738	0.43157	0.31288	0.40519	0.47842
3.10000	0.24124	0.02608	0.45598	0.36222	0.42553	0.52447
3.15000	0.31728	0.03790	0.48387	0.41628	0.43701	0.57330
3.20000	0.38199	0.05258	0.51137	0.47525	0.46389	0.62679
3.25000	0.43200	0.06971	0.54668	0.54027	0.47960	0.68383
3.30000	0.49678	0.09001	0.56022	0.60897	0.50471	0.74572
3.35000	0.55411	0.11335	0.59056	0.68360	0.53287	0.81306
3.40000	0.61303	0.13995	0.61063	0.76309	0.56006	0.88597

F. Ammonia/ammonia radial distribution function

R	g(NN)	INT(NN)	g(NH)	INT(NH)	g(HH)	INT(HH)
3.45000	0.69403	0.17096	0.61499	0.84552	0.57884	0.96355
3.50000	0.72960	0.20451	0.63563	0.93320	0.60967	1.04765
3.55000	0.75875	0.24040	0.64827	1.02519	0.61899	1.13549
3.60000	0.78820	0.27874	0.66776	1.12264	0.63933	1.22879
3.65000	0.79875	0.31869	0.67372	1.22372	0.65595	1.32720
3.70000	0.80048	0.35982	0.69333	1.33060	0.67056	1.43057
3.75000	0.82651	0.40345	0.69890	1.44127	0.68813	1.53954
3.80000	0.83962	0.44895	0.72335	1.55889	0.70695	1.65449
3.85000	0.85330	0.49643	0.73755	1.68199	0.72689	1.77581
3.90000	0.88250	0.54681	0.75776	1.81178	0.74054	1.90265
3.95000	0.88807	0.59882	0.77047	1.94714	0.75274	2.03490
4.00000	0.88964	0.65225	0.79706	2.09075	0.77128	2.17386
4.05000	0.89337	0.70725	0.80603	2.23963	0.78672	2.31917
4.10000	0.91459	0.76456	0.82122	2.39507	0.80150	2.47088
4.15000	0.93660	0.82551	0.83159	2.55635	0.82132	2.63017
4.20000	0.94582	0.88813	0.84527	2.72425	0.83798	2.79662
4.25000	0.96658	0.95367	0.86621	2.90043	0.85712	2.97096
4.30000	0.98874	1.02229	0.88626	3.08496	0.87623	3.15339
4.35000	0.99054	1.09264	0.90308	3.27739	0.89624	3.34436
4.40000	0.98798	1.16444	0.91547	3.47697	0.91794	3.54448
4.45000	0.99136	1.23812	0.93967	3.68650	0.94330	3.75483
4.50000	0.97980	1.31260	0.95155	3.90348	0.96211	3.97421
4.55000	1.00107	1.39039	0.96802	4.12915	0.98403	4.20361
4.60000	1.00205	1.46997	0.97861	4.36233	0.99815	4.44144
4.65000	1.03563	1.55403	0.98663	4.60256	1.01223	4.68791
4.70000	1.04789	1.64091	0.99970	4.85123	1.03036	4.94420
4.75000	1.05168	1.72998	1.02424	5.11145	1.04346	5.20931
4.80000	1.07764	1.82317	1.03898	5.38101	1.05463	5.48293
4.85000	1.09660	1.92000	1.05881	5.66147	1.06983	5.76630
4.90000	1.10082	2.01920	1.07670	5.95257	1.08690	6.06016
4.95000	1.12129	2.12233	1.08704	6.25250	1.09309	6.36176
5.00000	1.10237	2.22577	1.10932	6.56479	1.10234	6.67209
5.05000	1.09781	2.33086	1.11965	6.88633	1.11355	6.99187
5.10000	1.09463	2.43773	1.12847	7.21684	1.11735	7.31913
5.15000	1.08944	2.54619	1.14303	7.55822	1.12245	7.65436
5.20000	1.07441	2.65523	1.16486	7.91290	1.13334	7.99945
5.25000	1.06581	2.76550	1.17877	8.27876	1.13776	8.35258
5.30000	1.06329	2.87761	1.19743	8.65752	1.13662	8.71210

F. Ammonia/ammonia radial distribution function

R	g(NN)	INT(NN)	g(NH)	INT(NH)	g(HH)	INT(HH)
5.35000	1.06295	2.99181	1.20302	9.04526	1.14172	9.08009
5.40000	1.08974	3.11108	1.21764	9.44508	1.13677	9.45336
5.45000	1.09701	3.23339	1.23118	9.85687	1.14201	9.83532
5.50000	1.11068	3.35950	1.23360	10.27708	1.14930	10.22681
5.55000	1.15457	3.49299	1.24549	10.70909	1.14889	10.62531
5.60000	1.19280	3.63339	1.23533	11.14532	1.15317	11.03254
5.65000	1.22457	3.78012	1.22960	11.58732	1.16230	11.45034
5.70000	1.26033	3.93382	1.22551	12.03569	1.16620	11.87700
5.75000	1.30584	4.09588	1.22420	12.49146	1.16247	12.30980
5.80000	1.33213	4.26409	1.21743	12.95263	1.16481	12.75104
5.85000	1.37679	4.44094	1.20978	13.41884	1.16465	13.19985
5.90000	1.37442	4.62052	1.20765	13.89222	1.16791	13.65765
5.95000	1.40034	4.80661	1.20273	14.37170	1.17168	14.12475
6.00000	1.43292	5.00024	1.20567	14.86045	1.17015	14.59911
6.05000	1.42555	5.19609	1.19476	15.35289	1.17076	15.08166
6.10000	1.42115	5.39458	1.18547	15.84961	1.15676	15.56635
6.15000	1.39301	5.59234	1.17285	16.34912	1.14375	16.05347
6.20000	1.37619	5.79091	1.16655	16.85406	1.13697	16.54561
6.25000	1.35071	5.98895	1.16131	17.36488	1.12372	17.03989
6.30000	1.32846	6.18686	1.14624	17.87717	1.11002	17.53598
6.35000	1.27201	6.37938	1.14084	18.39516	1.10477	18.03760
6.40000	1.23524	6.56930	1.13120	18.91690	1.09386	18.54211
6.45000	1.18988	6.75510	1.11795	19.44061	1.07796	19.04710
6.50000	1.15944	6.93898	1.10596	19.96678	1.06596	19.55424
6.55000	1.13844	7.12231	1.09726	20.49687	1.05309	20.06299
6.60000	1.10881	7.30360	1.08103	21.02713	1.04754	20.57681
6.65000	1.07983	7.48284	1.07381	21.56186	1.03955	21.09448
6.70000	1.04583	7.65906	1.06008	22.09772	1.02790	21.61406
6.75000	1.00126	7.83030	1.03465	22.62856	1.01302	22.13379
6.80000	0.98114	8.00059	1.01899	23.15913	1.00097	22.65498
6.85000	0.94759	8.16748	0.99525	23.68500	0.98769	23.17685
6.90000	0.90790	8.32973	0.97805	24.20934	0.97984	23.70215
6.95000	0.87000	8.48746	0.96059	24.73181	0.97333	24.23155
7.00000	0.85333	8.64441	0.93991	25.25043	0.96337	24.76311
7.05000	0.83971	8.80107	0.92291	25.76695	0.96261	25.30185
7.10000	0.82553	8.95727	0.91225	26.28477	0.95219	25.84235
7.15000	0.81755	9.11415	0.89616	26.80066	0.94659	26.38727
7.20000	0.81454	9.27265	0.88915	27.31969	0.93773	26.93466

F. Ammonia/ammonia radial distribution function

R	g(NN)	INT(NN)	g(NH)	INT(NH)	g(HH)	INT(HH)
7.25000	0.81678	9.43379	0.88000	27.84055	0.92916	27.48462
7.30000	0.80850	9.59551	0.87612	28.36627	0.92442	28.03934
7.35000	0.81151	9.76007	0.86792	28.89424	0.91532	28.59615
7.40000	0.79903	9.92430	0.85854	29.42363	0.91410	29.15981
7.45000	0.78760	10.08839	0.85181	29.95599	0.90441	29.72505
7.50000	0.78076	10.25323	0.84696	30.49246	0.89352	30.29102
7.55000	0.79537	10.42341	0.84646	31.03578	0.88520	30.85921
7.60000	0.79107	10.59492	0.83955	31.58183	0.87755	31.42998
7.65000	0.81089	10.77305	0.83580	32.13261	0.87148	32.00427
7.70000	0.80974	10.95325	0.83723	32.69157	0.87099	32.58577
7.75000	0.81045	11.13597	0.83763	33.25809	0.86481	33.17067
7.80000	0.79444	11.31739	0.84089	33.83417	0.86282	33.76178
7.85000	0.80513	11.50362	0.84096	34.41771	0.86527	34.36220
7.90000	0.80273	11.69166	0.84727	35.01314	0.86411	34.96947
7.95000	0.81543	11.88511	0.84995	35.61804	0.86782	35.58708
8.00000	0.80772	12.07914	0.85061	36.23105	0.86861	36.21306
8.05000	0.80347	12.27458	0.84981	36.85117	0.87031	36.84813
8.10000	0.80763	12.47347	0.85251	37.48100	0.87141	37.49193
8.15000	0.81368	12.67634	0.85600	38.12125	0.86805	38.14119
8.20000	0.82064	12.88346	0.85437	38.76814	0.86895	38.79912
8.25000	0.82258	13.09361	0.85275	39.42171	0.87080	39.46651
8.30000	0.84127	13.31114	0.85682	40.08638	0.87257	40.14339
8.35000	0.84526	13.53235	0.86183	40.76302	0.87266	40.82852
8.40000	0.85388	13.75850	0.86782	41.45253	0.87104	41.52060
8.45000	0.84658	13.98539	0.87260	42.15413	0.87188	42.22162
8.50000	0.84996	14.21590	0.87159	42.86324	0.86792	42.92773
8.55000	0.85314	14.44999	0.87435	43.58298	0.86711	43.64151
8.60000	0.85451	14.68733	0.87706	44.31342	0.87089	44.36681
8.65000	0.86044	14.92898	0.87999	45.05484	0.86993	45.09975
8.70000	0.87236	15.17682	0.88548	45.80954	0.87304	45.84384
8.75000	0.88680	15.43167	0.88557	46.57301	0.87419	46.59752
8.80000	0.89967	15.69318	0.88660	47.34615	0.87144	47.35742
8.85000	0.91190	15.96127	0.88999	48.13107	0.86895	48.12379
8.90000	0.91718	16.23395	0.88644	48.92174	0.87207	48.90163
8.95000	0.93454	16.51492	0.88673	49.72156	0.87786	49.68443
9.00000	0.93454	16.88292	0.88673	49.72156	0.87786	49.68443
9.05000	0.93454	17.19492	0.88673	49.72156	0.87786	49.68443
9.10000	0.93454	17.51492	0.88673	49.72156	0.87786	49.68443

F. Ammonia/ammonia radial distribution function

R	g(NN)	INT(NN)	g(NH)	INT(NH)	g(HH)	INT(HH)
9.15000	0.93454	17.85492	0.88673	49.72156	0.87786	49.68443
9.20000	0.93454	18.10492	0.88673	49.72156	0.87786	49.68443
9.25000	0.93454	18.47492	0.88673	49.72156	0.87786	49.68443
9.30000	0.93454	18.79492	0.88673	49.72156	0.87786	49.68443
9.35000	0.93454	19.03492	0.88673	49.72156	0.87786	49.68443
9.40000	0.93454	19.41492	0.88673	49.72156	0.87786	49.68443
9.45000	0.93454	19.72492	0.88673	49.72156	0.87786	49.68443
9.50000	0.93454	20.06492	0.88673	49.72156	0.87786	49.68443
9.55000	0.93454	20.37492	0.88673	49.72156	0.87786	49.68443
9.60000	0.93454	20.74492	0.88673	49.72156	0.87786	49.68443
9.65000	0.93454	21.05492	0.88673	49.72156	0.87786	49.68443
9.70000	0.93454	21.41492	0.88673	49.72156	0.87786	49.68443
9.75000	0.93454	21.72492	0.88673	49.72156	0.87786	49.68443
9.80000	0.93454	22.08492	0.88673	49.72156	0.87786	49.68443
9.85000	0.93454	22.43492	0.88673	49.72156	0.87786	49.68443
9.90000	0.93454	22.76492	0.88673	49.72156	0.87786	49.68443
9.95000	0.93454	23.09492	0.88673	49.72156	0.87786	49.68443
10.00000	0.93454	23.48492	0.88673	49.72156	0.87786	49.68443

APPENDIX II : PROGRAM RADIAL DISTRIBUTION FUNCTIONS

```
      PROGRAM RADIAL                                                    LNR00010
C     ************************************************                  LNR00030
C     *     THIS PROGRAM CALCULATES RDF(S) AND THEIR    *
C     *     INTEGRAL FROM FILE KONSOUT (FOR Li-AMMONIA ) *              LNR00040
C     ************************************************
      INTEGER MSTEP                                                     LNR00050
      PARAMETER ( MSTEP=200, VIERPI=4.0*3.14159 )                       LNR00060
      INTEGER LLVEK(0:MSTEP),LHVEK(0:MSTEP),LOVEK(0:MSTEP),             LNR00090
     +LNVEK(0:MSTEP),LAVEK(0:MSTEP),HHVEK(0:MSTEP),OHVEK(0:MSTEP),      LNR00100
     +OOVEK(0:MSTEP),HNVEK(0:MSTEP),HAVEK(0:MSTEP),ONVEK(0:MSTEP),      LNR00110
     +OAVEK(0:MSTEP),NAVEK(0:MSTEP),NNVEK(0:MSTEP),AAVEK(0:MSTEP)       LNR00120
      REAL LADENS,LNDENS,FAKTOR                                         LNR00140
      REAL RLNVEK(0:MSTEP),RLAVEK(0:MSTEP),                             LNR00150
     +     X(0:MSTEP),                                                  LNR00160
     +     INTLN(0:MSTEP),INTLA(0:MSTEP)                                LNR00170
      CHARACTER LINE*80,RDFFMT*40,HEADER*80                             LNR00190
      INTEGER SEED                                                      LNR00210
      INTEGER MOZAHL,NION1,NION2,STEPS,NSTART,WAZALP,NION1P,            LNR00220
     +     NION2P,WAZAHL                                                LNR00230
      REAL ELDIM,ELDIMP,AUFLOE,AUFLOP                                   LNR00240
      NAMELIST /PARAM/SEED,NSTART,ELDIMP,MOZALP,NION1P,NION2P,          LNR00250
     +          WAZALP,RDFFMT,AUFLOP,HEADER                           LNR00260
      DATA RDFFMT /'(X,F6.2,7I8/7X,8I8)'/                               LNR00290
C     ************************************************************      LNR00300
      OPEN(10,FILE='INPRDF')                                            LNR00350
      OPEN(9,FILE='RDF')                                                LNR00360
      REWIND 10                                                         LNR00370
      READ(10,PARAM,END=444)                                            LNR00380
      ELDIM=ELDIMP                                                      LNR00390
      WAZAHL=WAZALP                                                     LNR00400
      AUFLOE=AUFLOP                                                     LNR00410
      MOZAHL=MOZALP                                                     LNR00420
      NION1=NION1P                                                      LNR00430
      NION2=NION2P                                                      LNR00440
      STEPS=9.0/AUFLOE                                                  LNR00450
      GOTO 555                                                          LNR00460
  444 CONTINUE                                                          LNR00470
      WRITE(*,*) ' *** SPECIFICATING PARAM - LIST NOT FOUND ***'        LNR00480
      GOTO 400                                                          LNR00490
```

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555 CONTINUE                                                          LNR00500
    WRITE(*,PARAM)                                                    LNR00510
    REWIND 10                                                         LNR00520
111 CONTINUE                                                          LNR00530
    READ(10,'(A)',END=222) LINE                                       LNR00540
    IF ( INDEX(LINE,'RDV') .EQ. 0 ) GOTO 111                          LNR00550
    GOTO 333                                                          LNR00560
222 CONTINUE                                                          LNR00570
    WRITE(*,*) ' *** START OF THE RDF - TABLE HAS NOT BEEN FOUND ***' LNR00580
    GOTO 400                                                          LNR00590
333 CONTINUE                                                          LNR00600
    READ(10,RDFFMT,ERR=400,END=55)                                    LNR00610
   +         (X(I),LLVEK(I),LHVEK(I),LOVEK(I),                        LNR00620
   +LNVEK(I),LAVEK(I),HHVEK(I),OHVEK(I),                              LNR00630
   +OOVEK(I),HNVEK(I),HAVEK(I),ONVEK(I),                              LNR00640
   +OAVEK(I),NAVEK(I),NNVEK(I),AAVEK(I),I=0,MSTEP)                    LNR00650
 55 CONTINUE                                                          LNR00720
    ELDIM=ELDIMP                                                      LNR00730
    WAZAHL=WAZALP                                                     LNR00740
    LNDENS = ELDIM**3*MOZAHL/(2*NION1*NION2*VIERPI*AUFLOE*NSTART)     LNR00760
    LADENS = ELDIM**3*MOZAHL/(6*NION1*NION2*VIERPI*AUFLOE*NSTART)     LNR00770
    RLNVEK(0)= 0.0                                                    LNR00790
    RLAVEK(0)= 0.0                                                    LNR00800
    INTLN(0) = 0.0                                                    LNR00820
    INTLA(0) = 0.0                                                    LNR00830
    DO 200, I=1,STEPS                                                 LNR00840
       RLNVEK(I) = REAL(LNVEK(I))*LNDENS/(REAL(I)*AUFLOE)**2          LNR00860
       RLAVEK(I) = REAL(LAVEK(I))*LADENS/(REAL(I)*AUFLOE)**2          LNR00870
       INTLN(I)=VIERPI*(REAL(I)*AUFLOE)**2*RLNVEK(I)*AUFLOE*NION1/    LNR00890
   +       ELDIM**3 + INTLN(I-1)                                      LNR00900
       INTLA(I)=VIERPI*(REAL(I)*AUFLOE)**2*RLAVEK(I)*AUFLOE*NION1*3/  LNR00910
   +       ELDIM**3 + INTLA(I-1)                                      LNR00920
200 CONTINUE                                                          LNR00940
    WRITE(9,'(/A//,2A//,(5F10.5))') '  NORMALIZED DENSITY VECTOR :',   LNR00960
   + '  DISTANCE      L-N    INTEGRAL   ',                            LNR00970
   + 'L-A    INTEGRAL                  ',                            LNR00980
   +(X(I),RLNVEK(I),INTLN(I),RLAVEK(I),INTLA(I),I=0,STEPS)            LNR00990
    STOP 'FINISHED'                                                   LNR01020
400 CONTINUE                                                          LNR01030
    STOP  ' CHECK INPRDF FILES'                                       LNR01040
    END                                                               LNR01050
```

APPENDIX III: PROGRAM DISTRIBUTION COORDINATION NUMBERS

```
      PROGRAM DISCN                                                     DIS00010
C ***************************************************************     DIS00020
C THIS PROGRAM CALCULATES THE DISTRIBUTION COORDINATION NUMBER          DIS00030
C FROM THE HISTORY FILES (WATER,AMMONIA AROUND LITHIUM ION)             DIS00040
C ***************************************************************     DIS00050
C ******FOR LITHIUM-WATER AND LITHIUM-AMMONIA *******                   DIS00060
      INTEGER MOZAHL,N,LO,LN,NUMLO(30),NUMLN(30)                        DIS00080
      REAL PLO(30),PLN(30)
      PARAMETER (MOZAHL = 202)                                          DIS00090
      INTEGER SPEC(MOZAHL),SPECI,SPECJ,MAX,NSET,TOTLO,TOTLN             DIS00100
      REAL RLO,RLN,RLH,RLA,R56                                          DIS00110
      REAL XKOORD(MOZAHL),YKOORD(MOZAHL),ZKOORD(MOZAHL)                 DIS00120
      REAL ALPHA(MOZAHL),BETA(MOZAHL),GAMMA(MOZAHL)                     DIS00130
      REAL MINLO,MINLN,X5,Y5,Z5,X6,Y6,Z6                                DIS00150
      CHARACTER LINE1*80,LINE2*80                                       DIS00170
      DATA MINLO,MINLN/2.75,3.80/                                       DIS00190
      DATA MAX/200/                                                     DIS00200
C     ***********************************************************       DIS00210
      OPEN(11,FILE='INPCN')                                             DIS00220
      OPEN(9,FILE='DISOUT')                                             DIS00230
      REWIND (11)                                                       DIS00240
          DO 5 I=1,30                                                   DIS00250
            NUMLO(I) = 0                                                DIS00260
            NUMLN(I) = 0                                                DIS00270
              PLO(I) = 0.0
              PLN(I) = 0.0
  5       CONTINUE                                                      DIS00280
       NSET = 0                                                         DIS00290
      TOTLO = 0                                                         DIS00300
      TOTLN = 0                                                         DIS00310
100   CONTINUE
      READ(11,'(A)') LINE1                                              DIS00320
      READ(11,'(A)') LINE2                                              DIS00330
      READ(11,'(5X,I5,6F10.5)')                                         DIS00350
     + (SPEC(I),XKOORD(I),YKOORD(I),ZKOORD(I),ALPHA(I),BETA(I),GAMMA(I),DIS00360
     + I=1,MOZAHL)                                                      DIS00370
      NSET=NSET+1                                                       DIS00440
      DO 10 I=1,MOZAHL                                                  DIS00450
            SPECI=SPEC(I)                                               DIS00460
```

```
          IF(SPECI.NE.3) GOTO 10                                          DIS00470
            X5 = XKOORD(I)                                                DIS00480
            Y5 = YKOORD(I)                                                DIS00490
            Z5 = ZKOORD(I)                                                DIS00500
            LO = 0                                                        DIS00520
            LN = 0                                                        DIS00530
               DO 20 J=1,MOZAHL                                           DIS00550
C *****COUNT NUMBER OF NITROGEN AND OXYGEN AROUND ATOM LITHIUM*****       DIS00560
               SPECJ=SPEC(J)                                              DIS00570
             IF(SPECJ.NE.3) THEN                                          DIS00580
               X6 = XKOORD(J)                                             DIS00590
               Y6 = YKOORD(J)                                             DIS00600
               Z6 = ZKOORD(J)                                             DIS00610
             ENDIF                                                        DIS00620
C                                                                         DIS00630
C *****CALCULATETHE DISTANCE BET Li-O AND Li-N ********                   DIS00640
      R56 = ((X6-X5)**2+(Y6-Y5)**2+(Z6-Z5)**2)                            DIS00660
C*****Li-O DISTANCE*****                                                  DIS00680
          IF(SPECJ.EQ.1.AND.R56.LE.MINLO*MINLO) LO=LO+1                   DIS00690
C*****Li-N DISTANCE*****                                                  DIS00700
          IF(SPECJ.EQ.2.AND.R56.LE.MINLN*MINLN) LN=LN+1                   DIS00710
 20               CONTINUE                                                DIS00720
          NUMLO(LO)=NUMLO(LO)+1                                           DIS00730
          NUMLN(LN)=NUMLN(LN)+1                                           DIS00740
 10    CONTINUE                                                           DIS00750
          IF (NSET.EQ.MAX) GOTO 200                                       DIS00760
      GOTO 100                                                            DIS00770
200       DO 15 J = 1,30
      TOTLO = TOTLO+NUMLO(J)
      TOTLN = TOTLN+NUMLN(J)
 15       CONTINUE
          DO 35 I = 1,30
      PLO(I)=NUMLO(I)*100.0/REAL(TOTLO)
      PLN(I)=NUMLN(I)*100.0/REAL(TOTLN)
 35       CONTINUE
      WRITE(9,'(9X,I5)') 'NSET=',NSET                                     DIS00810
      WRITE(9,*)'DISTRIBUTION OF COORDINATION NUMBER AROUND AN ATOM'      DIS00820
      WRITE(9,*) '    I          PLO(LO)          PLN(LN)'                DIS00830
      WRITE(9,'(3X,I3,8X,F8.2,9X,F8.2)') (I,PLO(I),PLN(I) , I=1,30)       DIS00840
      STOP 'FINISHED'                                                     DIS00850
      END                                                                 DIS00860
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ABPPENDIX IV: DISTRIBUTIONS OF ANGLES

```
C PROGRAM COSWA                                                        COS00010
C ************************************************************        COS00030
C THIS PROGRAM CALCULATES THE DISTRIBUTION OF THE ANGULAR              COS00040
C OF WATER AROUND LITHIUM ION FROM THE HISTORY FILES                   COS00050
C ************************************************************        COS00060
C                                                                      COS00070
      INTEGER MOZAHL,NSET,MAX,ICOSW,KCOSW,TOTCOS                       COS00080
      PARAMETER (MOZAHL = 202)                                         COS00090
      PARAMETER (ICOSW = 201)                                          COS00100
      INTEGER SPEC(MOZAHL),SPECI,SPECJ,ICOS(ICOSW)                     COS00110
      REAL ABSA,ABSB,R56,COSW,VECAB,A(201),PCOS(201)                   COS00120
      REAL AUFLOE,MAXDIS,MINDIS                                        COS00130
      PARAMETER (AUFLOE=0.05)                                          COS00140
      REAL   XKOORD (MOZAHL),                                          COS00150
     +       YKOORD (MOZAHL),                                          COS00160
     +       ZKOORD (MOZAHL),                                          COS00170
     +       ALPHA (MOZAHL),                                           COS00180
     +       BETA  (MOZAHL),                                           COS00190
     +       GAMMA (MOZAHL)                                            COS00200
      REAL HNX,HNY,HNZ                                                 COS00210
      REAL ALP,BET,GAM,H1X,H1Y,H1Z,H2X,H2Y,H2Z,H7X,H7Y,H7Z,X5,Y5,Z5,   COS00220
     +XAM,YAM,ZAM,X6,Y6,Z6,H3X,H3Y,H3Z,H4X,H4Y,H4Z,H8X,H8Y,H8Z         COS00230
      REAL SINALP,SINBET,SINGAM,COSALP,COSBET,COSGAM,                  COS00240
     +          A11,A12,A13,A21,A22,A23,A31,A32,A33                    COS00250
      REAL YH1ST,YH2ST,ZHST,ZMST                                       COS00260
      CHARACTER LINE1*80,LINE2*80                                      COS00270
      DATA MINDIS,MAXDIS/0.0,2.75/                                     COS00280
      MAX = 200                                                        COS00290
      YH1ST=0.75669                                                    COS00300
      YH2ST=-0.75669                                                   COS00310
      ZHST=0.58589                                                     COS00320
      ZMST=0.2677                                                      COS00330
      OPEN(11,FILE='SAMHIS')                                           COS00340
      OPEN(9,FILE='WACOS')                                             COS00350
      NSET=0                                                           COS00360
      TOTCOS=0                                                         COS00370
      DO 11 K=1,201                                                    COS00380
           PCOS(K)=0.0                                                 COS00390
           ICOS(K)=0                                                   COS00400
```

```
 11   CONTINUE                                                          COS00410
C ***************************************************************      COS00420
C     WRITE(*,*) 'HAVE YOU ALREADY CHECKED THE MAX-DISTANCE ?'          COS00440
 100  CONTINUE                                                          COS00460
      READ(11,'(A)') LINE1                                              COS00470
      READ(11,'(A)') LINE2                                              COS00480
      READ(11,'(5X,I5,6F10.5)',END=222) (SPEC(I),XKOORD(I),YKOORD(I),   COS00490
     +       ZKOORD(I),ALPHA(I),BETA(I),GAMMA(I),I=1,MOZAHL)            COS00500
      NSET = NSET+1                                                     COS00510
      DO 10 I=1,MOZAHL                                                  COS00520
      SPECI = SPEC(I)                                                   COS00530
      IF (SPECI.NE.3) GOTO 10                                           COS00540
      X5 = XKOORD(I)                                                    COS00550
      Y5 = YKOORD(I)                                                    COS00560
      Z5 = ZKOORD(I)                                                    COS00570
      KCOS = 0                                                          COS00590
           DO 20 J=1,MOZAHL                                             COS00600
C **********DIPOLE  VECTOR********                                      COS00610
           SPECJ = SPEC(J)                                              COS00620
             IF (SPECJ.EQ.1) THEN                                       COS00630
              X6 = XKOORD(J)                                            COS00640
              Y6 = YKOORD(J)                                            COS00650
              Z6 = ZKOORD(J)                                            COS00660
              ALP=ALPHA(J)                                              COS00670
              BET=BETA(J)                                               COS00680
              GAM=GAMMA(J)                                              COS00690
           SINALP=SIN(ALP)                                              COS00730
           COSALP=COS(ALP)                                              COS00740
           SINBET=SIN(BET)                                              COS00750
           COSBET=COS(BET)                                              COS00760
           SINGAM=SIN(GAM)                                              COS00770
           COSGAM=COS(GAM)                                              COS00780
      A21=COSALP*SINGAM+SINALP*SINBET*COSGAM                            COS00800
      A22=COSALP*COSGAM-SINALP*SINBET*SINGAM                            COS00810
      A23=-SINALP*COSBET                                                COS00820
      A31=SINALP*SINGAM-COSALP*SINBET*COSGAM                            COS00830
      A32=SINALP*COSGAM+COSALP*SINBET*SINGAM                            COS00840
      A33=COSALP*COSBET                                                 COS00850
      H1X=A21*YH1ST+A31*ZHST + X6                                       COS00870
      H1Y=A22*YH1ST+A32*ZHST + Y6                                       COS00880
      H1Z=A23*YH1ST+A33*ZHST + Z6                                       COS00890
```

```
      H2X=A21*YH2ST+A31*ZHST + X6                                        COS00900
      H2Y=A22*YH2ST+A32*ZHST + Y6                                        COS00910
      H2Z=A23*YH2ST+A33*ZHST + Z6                                        COS00920
      M7X=A31*ZMST + X6                                                  COS00930
      M7Y=A32*ZMST + Y6                                                  COS00940
      M7Z=A33*ZMST + Z6                                                  COS00950
      HNX=(H1X+H2X)/2.0                                                  COS00970
      HNY=(H1Y+H2Y)/2.0                                                  COS00980
      HNZ=(H1Z+H2Z)/2.0                                                  COS00990
      R56 = SQRT((X6-X5)**2+(Y6-Y5)**2+(Z6-Z5)**2)                       COS01040
      IF (R56.GE.MINDIS.AND.R56.LE.MAXDIS) THEN                          COSC1050
      DH1 = SQRT((HNX-H1X)**2+(HNY-H1Y)**2+(HNZ-H1Z)**2)                 COSC1080
      DH2 = SQRT((HNX-H2X)**2+(HNY-H2Y)**2+(HNZ-H2Z)**2)                 COS01090
      VECAB = (X5-X6)*(HNX-X6)                                           COS01120
     +       +(Y5-Y6)*(HNY-Y6)                                           COS01130
     +       +(Z5-Z6)*(HNZ-Z6)                                           COS01140
      ABSA = R56                                                         COS01160
      ABSB = SQRT((X6-HNX)**2+(Y6-HNY)**2+(Z6-HNZ)**2)                   COS01170
      COSW = VECAB/(ABSA*ABSB)                                           COS01190
      KCOSW = COSW*100+101                                               COS01200
      ICOS(KCOSW) = ICOS(KCOSW)+1                                        COS01210
      ENDIF                                                              COS01220
            ENDIF                                                        COS01230
20                CONTINUE                                               COS01260
10    CONTINUE                                                           COS01270
      IF (NSET.EQ.MAX) GOTO 200                                          COS01290
      GOTO 100                                                           COS01300
222    CONTINUE                                                          COS01320
200    DO 33 M=1,201                                                     COS01340
       A(M) =(M-101)/100.0                                               COS01350
       TOTCOS=TOTCOS+ICOS(M)                                             COS01360
33     CONTINUE                                                          COS01370
       WRITE(*,*) TOTCOS                                                 COS01380
       DO 35 M=1,201                                                     COS01390
       IF (ICOS(M).GT.0) PCOS(M)=REAL(ICOS(M)/REAL(TOTCOS))              COS01400
35     CONTINUE                                                          COS01410
      WRITE(9,'(9X,I5)')'NSET=',NSET                                     COS01440
      WRITE(9,*)'    A(M)        PCOSW(M)      ICOS(M)'                  COS01450
      WRITE(9,'(1X,F8.2,5X,F9.4,3X,I8)')(A(M),PCOS(M),ICOS(M),M=1,201)   COS01460
      STOP 'FINISHED'                                                    COS01480
      END                                                                COS01490
```

APPENDIX V : DISTRIBUTIONS OF ANGLES

```
C PROGRAM COSAM                                                        COS00010
C                                                                      COS00020
C ***************************************************************      COS00030
C THIS PROGRAM CALCULATES THE DISTRIBUTION OF THE ANGULAR              COS00040
C OF WATER AROUND LITHIUM ION FROM THE HISTORY FILES                   COS00050
C ***************************************************************      COS00060
C                                                                      COS00070
      INTEGER MOZAHL,NSET,MAX,ICOSW,KCOSW,TOTCOS                       COS00080
      PARAMETER (MOZAHL = 202)                                         COS00090
      PARAMETER (ICOSW = 201)                                          COS00100
      INTEGER SPEC(MOZAHL),SPECI,SPECJ,ICOS(ICOSW)                     COS00110
      REAL ABSA,ABSB,R56,COSW,VECAB,A(201),PCOS(201)                   COS00120
      REAL AUFLOE,MAXDIS,MINDIS                                        COS00130
      PARAMETER (AUFLOE=0.05)                                          COS00140
      REAL   XKOORD (MOZAHL),                                          COS00150
     +       YKOORD (MOZAHL),                                          COS00160
     +       ZKOORD (MOZAHL),                                          COS00170
     +       ALPHA (MOZAHL),                                           COS00180
     +       BETA  (MOZAHL),                                           COS00190
     +       GAMMA (MOZAHL)                                            COS00200
      REAL YH1AM,YH2AM,ZHAM,ZMAM,XCAM,ZCAM,HNX,HNY,HNZ                 COS00210
      REAL ALP,BET,GAM,H1X,H1Y,H1Z,H2X,H2Y,H2Z,H7X,H7Y,H7Z,X5,Y5,Z5,   COS00220
     +XAM,YAM,ZAM,X6,Y6,Z6,H3X,H3Y,H3Z,H4X,H4Y,H4Z,H8X,H8Y,H8Z         COS00230
      REAL SINALP,SINBET,SINGAM,COSALP,COSBET,COSGAM,                  COS00240
     +          A11,A12,A13,A21,A22,A23,A31,A32,A33                    COS00250
      CHARACTER LINE1*80,LINE2*80                                      COS00260
      DATA MINDIS,MAXDIS/0.0,3.0/                                      COS00270
      MAX = 200                                                        COS00280
      YH1AM=0.81209                                                    COS00290
      YH2AM=-0.81225                                                   COS00300
      ZHAM=0.60454                                                     COS00310
      ZMAM=-0.48611                                                    COS00320
      XMAM=-0.88806                                                    COS00330
      XCAM=-0.11950                                                    COS00340
      ZCAM=0.10030                                                     COS00350
      OPEN(11,FILE='SAMHIS')                                           COS00360
      OPEN(9,FILE='AMCOS')                                             COS00370
      NSET=0                                                           COS00380
```

```
      TOTCOS=0                                                          COS00390
      DO 11 K=1,201                                                     COS00400
           PCOS(K)=0.0                                                  COS00410
           ICOS(K)=0                                                    COS00420
 11   CONTINUE                                                          COS00430
C ******************************************************************** COS00440
C                                                                       COS00450
C     WRITE(*,*) 'HAVE YOU ALREADY CHECKED THE MAX-DISTANCE ?'          COS00460
C     WRITE(*,*) 'IF EVERYTHING O.K , I HOPE YOU WILL "GOOD-LUCK".'     COS00470
 100  CONTINUE                                                          COS00480
      READ(11,'(A)') LINE1                                              COS00490
      READ(11,'(A)') LINE2                                              COS00500
      READ(11,'(5X,I5,6F10.5)',END=222) (SPEC(I),XKOORD(I),YKOORD(I),   COS00510
     +       ZKOORD(I),ALPHA(I),BETA(I),GAMMA(I),I=1,MOZAHL)            COS00520
      NSET = NSET+1                                                     COS00530
      DO 10 I=1,MOZAHL                                                  COS00540
      SPECI = SPEC(I)                                                   COS00550
      IF (SPECI.NE.3) GOTO 10                                           COS00560
      X5 = XKOORD(I)                                                    COS00570
      Y5 = YKOORD(I)                                                    COS00580
      Z5 = ZKOORD(I)                                                    COS00590
C                                                                       COS00600
           KCOS = 0                                                     COS00610
           DO 20 J=1,MOZAHL                                             COS00620
C **********DIPOLE  VECTOR********                                      COS00630
C
           SPECJ = SPEC(J)                                              COS00640
      IF (SPECJ.EQ.2) THEN                                              COS00650
              X6 = XKOORD(J)                                            COS00660
              Y6 = YKOORD(J)                                            COS00670
              Z6 = ZKOORD(J)                                            COS00680
              ALP=ALPHA(J)                                              COS00690
              BET=BETA(J)                                               COS00700
              GAM=GAMMA(J)                                              COS00710
C                                                                       COS00720
           SINALP=SIN(ALP)                                              COS00750
           COSALP=COS(ALP)                                              COS00760
           SINBET=SIN(BET)                                              COS00770
           COSBET=COS(BET)                                              COS00780
           SINGAM=SIN(GAM)                                              COS00790
           COSGAM=COS(GAM)                                              COS00800
```

```
      A11=COSBET*COSGAM                                                 COS00820
      A12=-COSBET*SINGAM                                                COS00830
      A13=SINBET                                                        COS00840
      A21=COSALP*SINGAM+SINALP*SINBET*COSGAM                            COS00850
      A22=COSALP*COSGAM-SINALP*SINBET*SINGAM                            COS00860
      A23=-SINALP*COSBET                                                COS00870
      A31=SINALP*SINGAM-COSALP*SINBET*COSGAM                            COS00880
      A32=SINALP*COSGAM+COSALP*SINBET*SINGAM                            COS00890
      A33=COSALP*COSBET                                                 COS00900
C                                                                       COS00910
      H3X=A21*YH1AM+A31*ZHAM + X6                                       COS00940
      H3Y=A22*YH1AM+A32*ZHAM + Y6                                       COS00950
      H3Z=A23*YH1AM+A33*ZHAM + Z6                                       COS00960
      H4X=A21*YH2AM+A31*ZHAM + X6                                       COS00970
      H4Y=A22*YH2AM+A32*ZHAM + Y6                                       COS00980
      H4Z=A23*YH2AM+A33*ZHAM + Z6                                       COS00990
      H8X=A11*XMAM+A31*ZMAM + X6                                        COS01000
      H8Y=A12*XMAM+A32*ZMAM + Y6                                        COS01010
      H8Z=A13*XMAM+A33*ZMAM + Z6                                        COSC1020
C                                                                       COSC1030
      HNX=(H3X+H4X+H8X)/3.0                                             COSC1040
      HNY=(H3Y+H4Y+H8Y)/3.0                                             COSC1050
      HNZ=(H3Z+H4Z+H8Z)/3.0                                             COSC1060
C
      R56 = SQRT((X6-X5)**2+(Y6-Y5)**2+(Z6-Z5)**2)                      COSC1110
      IF (R56.GE.MINDIS.AND.R56.LE.MAXDIS) THEN                         COSC1120
C
      DH1 = SQRT((HNX-H3X)**2+(HNY-H3Y)**2+(HNZ-H3Z)**2)                COS01140
      DH2 = SQRT((HNX-H4X)**2+(HNY-H4Y)**2+(HNZ-H4Z)**2)                COS01150
      DH3 = SQRT((HNX-H8X)**2+(HNY-H8Y)**2+(HNZ-H8Z)**2)                COS01160
C                                                                       COS01170
      VECAB = (X6-X5)*(HNX-X6)                                          COS01180
     +       +(Y6-Y5)*(HNY-Y6)                                          COS01190
     +       +(Z6-Z5)*(HNZ-Z6)                                          COS01200

      ABSA = R56                                                        COS01220
      ABSB = SQRT((X6-HNX)**2+(Y6-HNY)**2+(Z6-HNZ)**2)                  COS01230
C                                                                       COS01240
      COSW = VECAB/(ABSA*ABSB)                                          COS01250
      KCOSW = COSW*100+101                                              COS01260
      ICOS(KCOSW) = ICOS(KCOSW)+1                                       COS01270
```

```
      ENDIF                                                              COS01280
      ENDIF                                                              COS01290
C                                                                        COS01300
 20                CONTINUE                                             COS01320
 10   CONTINUE                                                           COS01330
C                                                                        COS01340
      IF (NSET.EQ.MAX) GOTO 201                                          COS01350
      GOTO 100                                                           COS01360
C                                                                        COS01370
 222   CONTINUE                                                          COS01380
C                                                                        COS01390
 201   DO 33 M=1,201                                                     COS01400
       A(M) =(M-101)/100.0                                              COS01410
       TOTCOS=TOTCOS+ICOS(M)                                            COS01420
 33    CONTINUE                                                          COS01430
       WRITE(*,*) TOTCOS                                                COS01440
       DO 35 M=1,201                                                    COS01450
       IF (ICOS(M).GT.0) PCOS(M)=REAL(ICOS(M)/REAL(TOTCOS))             COS01460
 35    CONTINUE                                                          COS01470
       WRITE(9,'(9X,I5)')'NSET=',NSET                                   COS01500
       WRITE(9,*)'    A(M)       PCOSW(I)       ICOS(I)'               COS01510
       WRITE(9,'(1X,F8.2,5X,F9.4,3X,I8)') (A(M),PCOS(M),ICOS(M),M=1,201)COS01520
      STOP 'FINISHED'                                                    COS01540
      END                                                                COS01550
```

APPENDIX VI: PROGRAM DISTRIBUTION OF ENERGIES

```
      PROGRAM DISENE                                                    LWE00010
C ***************************************************************     LWE00060
C THIS PROGRAM CALCULATES THE DISTRIBUTION OF THE ENERGIES              LWE00070
C OF WATER AND LITHIUM ION INTERACTION FROM THE HISTORY FILES           LWE00080
C ***************************************************************     LWE00090
      INTEGER MOZAHL,NSET,MAX,KE                                        LWE00110
      PARAMETER (MOZAHL = 202)                                          LWE00120
      INTEGER SPEC(MOZAHL),SPECI,SPECJ,IENER(121)                       LWE00130
      REAL R56,A(121),TOTAL,PDIST(121),E                                LWE00140
      REAL AUFLOE,MAXDIS,MINDIS                                         LWE00150
      PARAMETER (AUFLOE=0.05)                                           LWE00160
      REAL   XKOORD (MOZAHL),                                           LWE00170
     +       YKOORD (MOZAHL),                                           LWE00180
     +       ZKOORD (MOZAHL),                                           LWE00190
     +       ALPHA (MOZAHL),                                            LWE00200
     +       BETA  (MOZAHL),                                            LWE00210
     +       GAMMA (MOZAHL)                                             LWE00220
C
      REAL ALP,BET,GAM,H1X,H1Y,H1Z,H2X,H2Y,H2Z,H7X,H7Y,H7Z,X5,Y5,Z5,    LWE00230
     +XAM,YAM,ZAM,X6,Y6,Z6,H3X,H3Y,H3Z,H4X,H4Y,H4Z,H8X,H8Y,H8Z          LWE00240
      REAL SINALP,SINBET,SINGAM,COSALP,COSBET,COSGAM,                   LWE00250
     +          A11,A12,A13,A21,A22,A23,A31,A32,A33                     LWE00260
      REAL YH1ST,YH2ST,ZHST,ZMST                                        LWE00270
      CHARACTER LINE1*80,LINE2*80                                       LWE00280
      DATA MINDIS,MAXDIS/1.0,18.5285/                                   LWE00290
      MAX = 200                                                         LWE00300
      YH1ST=0.75669                                                     LWE00310
      YH2ST=-0.75669                                                    LWE00320
      ZHST=0.58589                                                      LWE00330
      ZMST=0.2677                                                       LWE00340
      OPEN(11,FILE='INPCOS')                                            LWE00350
      OPEN(9,FILE='DLWOUT')                                             LWE00360
      NSET=0                                                            LWE00370
      TOTAL=0.0                                                         LWE00380
      DO 11 K=1,121                                                     LWE00390
           PDIST(K)=0.0                                                 LWE00400
           IDIST(K)=0                                                   LWE00410
 11     CONTINUE                                                        LWE00420
```

```
100   CONTINUE                                                          LWE00450
      READ(11,'(A)') LINE1                                              LWE00460
      READ(11,'(A)') LINE2                                              LWE00470
      READ(11,'(5X,I5,6F10.5)',END=222) (SPEC(I),XKOORD(I),YKOORD(I),   LWE00480
     +       ZKOORD(I),ALPHA(I),BETA(I),GAMMA(I),I=1,MOZAHL)            LWE00490

C     NSET = NSET+1                                                     LWE00500
      DO 10 I=1,MOZAHL                                                  LWE00510
      SPECI = SPEC(I)                                                   LWE00520
      IF (SPECI.NE.3) GOTO 10                                           LWE00530

C     X5 = XKOORD(I)                                                    LWE00540
      Y5 = YKOORD(I)                                                    LWE00550
      Z5 = ZKOORD(I)                                                    LWE00560
      KE = 0
          DO 20 J=1,MOZAHL                                              LWE00580
C **********DIPOLE  VECTOR********                                      LWE00590
          SPECJ = SPEC(J)                                               LWE00600
            IF (SPECJ.EQ.1) THEN                                        LWE00610
             X6 = XKOORD(J)                                             LWE00620
             Y6 = YKOORD(J)                                             LWE00630
             Z6 = ZKOORD(J)                                             LWE00640
             ALP=ALPHA(J)                                               LWE00650
             BET=BETA(J)                                                LWE00660
             GAM=GAMMA(J)                                               LWE00670
C
          SINALP=SIN(ALP)                                               LWE00710
          COSALP=COS(ALP)                                               LWE00720
          SINBET=SIN(BET)                                               LWE00730
          COSBET=COS(BET)                                               LWE00740
          SINGAM=SIN(GAM)                                               LWE00750
          COSGAM=COS(GAM)                                               LWE00760
C
      A21=COSALP*SINGAM+SINALP*SINBET*COSGAM                            LWE00780
      A22=COSALP*COSGAM-SINALP*SINBET*SINGAM                            LWE00790
      A23=-SINALP*COSBET                                                LWE00800
      A31=SINALP*SINGAM-COSALP*SINBET*COSGAM                            LWE00810
      A32=SINALP*COSGAM+COSALP*SINBET*SINGAM                            LWE00820
      A33=COSALP*COSBET                                                 LWE00830
```

```
C########CALCULATE COORDINATE OF WATER MOLECULE##########                LWE00850
      H1X=A21*YH1ST+A31*ZHST + X6                                        LWE00870
      H1Y=A22*YH1ST+A32*ZHST + Y6                                        LWE00880
      H1Z=A23*YH1ST+A33*ZHST + Z6                                        LWE00890
      H2X=A21*YH2ST+A31*ZHST + X6                                        LWE00900
      H2Y=A22*YH2ST+A32*ZHST + Y6                                        LWE00910
      H2Z=A23*YH2ST+A33*ZHST + Z6                                        LWE00920
      M7X=A31*ZMST + X6                                                  LWE00930
      M7Y=A32*ZMST + Y6                                                  LWE00940
      M7Z=A33*ZMST + Z6                                                  LWE00950
C
      R56 = SQRT((X6-X5)**2+(Y6-Y5)**2+(Z6-Z5)**2)                       LWE00980
C########CALCULATE DISTANCE BETWEEN LITHIUM AND WATER MOLECULE######     LWE01010
C ** SPECI = LI  ; SPECJ = H2O**                                         LWE01030
      XREL7 = H1X-X5                                                     LWE01040
      YREL7 = H1Y-Y5                                                     LWE01050
      ZREL7 = H1Z-Z5                                                     LWE01060
      XREL8 = H2X-X5                                                     LWE01070
      YREL8 = H2Y-Y5                                                     LWE01080
      ZREL8 = H2Z-Z5                                                     LWE01090
C
      RH7 = SQRT(XREL7**2+YREL7**2+ZREL7**2)                             LWE01100
      RH8 = SQRT(XREL8**2+YREL8**2+ZREL8**2)                             LWE01110
C   ************************************                                 LWE01120
C     LITHIUM-WATER-POTENTIAL FUNCTION                                   LWE01130
C   ************************************                                 LWE01140
      E=0.0                                                              LWE01150
      E= (-15.22/R56+1499.0*EXP(-3.93*R56)-8.109/R56**2                  LWE01160
     + +7.609/RH7+191.0*EXP(-5.87*RH7)                                   LWE01170
     + +3.934/RH7**2                                                     LWE01180
     + +7.609/RH8+191.0*EXP(-5.87*RH8)                                   LWE01190
     + +3.934/RH8**2)*14.3836                                            LWE01200
C
         KE=E*2+81                                                       LWE01240
          IENER(KE)=IENER(KE)+1                                          LWE01260
C
       WRITE(*,*) 'IENER(KE)=',IENER(KE)                                 LWE01270
           ENDIF                                                         LWE01290
 20              CONTINUE                                                LWE01310
 10   CONTINUE                                                           LWE01320
```

```
      IF (NSET.EQ.MAX) GOTO 200                                          LWE01340
       GOTO 100                                                          LWE01350
222    CONTINUE                                                          LWE01370
200    DO 33 M=1,121                                                     LWE01390
       A(M)=(M-81.0)/2.0                                                 LWE01400
       TOTAL=TOTAL+IENER(M)                                              LWE01410
 33    CONTINUE                                                          LWE01420
C
       WRITE(*,*) 'TOTAL=',TOTAL                                         LWE01440
       DO 35 M=1,121                                                     LWE01450
       IF(IENER(M).GT.0) PDIST(M)=IENER(M)/TOTAL                         LWE01460
  35   CONTINUE                                                          LWE01470

C      WRITE(9,'(9X,I5)')'NSET=',NSET                                    LWE01500
       WRITE(9,'(9X,F10.5)')'TOTAL=',TOTAL                               LWE01510
       WRITE(9,*)'       A(M)          PDIST(M)'                         LWE01520
       WRITE(9,'(1X,F10.2,5X,F12.5)') ( A(M),PDIST(M),M=1,121)           LWE01530
C                                                                        LWE01540
       STOP 'FINISHED'                                                   LWE01550
       END                                                               LWE01560
```

APPENDIX VII : PROGRAM DISTRIBUTION OF ENERGIES

```
      PROGRAM DISENE                                                    LAE00010
C ***************************************************************     LAE00060
C THIS PROGRAM CALCULATES THE DISTRIBUTION OF THE ENERGIES              LAE00070
C OF AMMONIA AND LITHIUM ION INTERACTION FROM THE HISTORY FILES         LAE00080
C ***************************************************************     LAE00090
C                                                                       LAE00100
      INTEGER MOZAHL,NSET,MAX,KE                                        LAE00110
      PARAMETER (MOZAHL = 202)                                          LAE00120
      INTEGER SPEC(MOZAHL),SPECI,SPECJ,IENER(201)                       LAE00130
      REAL R56,A(201),TOTAL,PDIST(201),E                                LAE00140
      REAL MAXDIS,MINDIS                                                LAE00150
      REAL   XKOORD (MOZAHL),                                           LAE00160
     +       YKOORD (MOZAHL),                                           LAE00170
     +       ZKOORD (MOZAHL),                                           LAE00180
     +       ALPHA (MOZAHL),                                            LAE00190
     +       BETA  (MOZAHL),                                            LAE00200
     +       GAMMA (MOZAHL)                                             LAE00210
      REAL YH1AM,YH2AM,ZHAM,ZMAM,XCAM,ZCAM,HNX,HNY,HNZ                  LAE00220
      REAL ALP,BET,GAM,H1X,H1Y,H1Z,H2X,H2Y,H2Z,H7X,H7Y,H7Z,X5,Y5,Z5,    LAE00230
     +XAM,YAM,ZAM,X6,Y6,Z6,H4XA,H4YA,H4ZA,H8XA,H8YA,H8ZA,H10XA,         LAE00240
     +H10YA,H10ZA,H3XA,H3YA,H3ZA,ANGALU,ALUANG                          LAE00250
      REAL SINALP,SINBET,SINGAM,COSALP,COSBET,COSGAM,                   LAE00260
     +          A11,A12,A13,A21,A22,A23,A31,A32,A33                     LAE00270
      CHARACTER LINE1*80,LINE2*80                                       LAE00280
      DATA MINDIS,MAXDIS/1.0,26.21/                                     LAE00290
      YH1AM=0.81209                                                     LAE00300
      YH2AM=-0.81225                                                    LAE00310
      ZHAM=0.60454                                                      LAE00320
      ZMAM=-0.48611                                                     LAE00330
      XMAM=-0.88806                                                     LAE00340
      XCAM=-0.11950                                                     LAE00350
      ZCAM=0.10030                                                      LAE00360
      ALUANG=0.529167                                                   LAE00370
      ANGALU=1.8897626                                                  LAE00380
      MAX = 2                                                           LAE00390
      OPEN(11,FILE='INPCOS')                                            LAE00400
      OPEN(9,FILE='DLAOUT')                                             LAE00410
      NSET=0                                                            LAE00420
      TOTAL=0.0                                                         LAE00430
```

```
      DO 11 K=1,201                                                    LAE00440
        PDIST(K)=0.0                                                   LAE00450
        IENER(K)=0                                                     LAE00460
 11   CONTINUE                                                         LAE00470
C*********************************************************************LAE00480
C                                                                      LAE00490
 100  CONTINUE                                                         LAE00500
      READ(11,'(A)') LINE1                                             LAE00510
      READ(11,'(A)') LINE2                                             LAE00520
      READ(11,'(5X,I5,6F10.5)',END=222) (SPEC(I),XKOORD(I),YKOORD(I),  LAE00530
     +       ZKOORD(I),ALPHA(I),BETA(I),GAMMA(I),I=1,MOZAHL)           LAE00540
      NSET = NSET+1                                                    LAE00550
      DO 10 I=1,MOZAHL                                                 LAE00560
      SPECI = SPEC(I)                                                  LAE00570
      IF (SPECI.NE.3) GOTO 10                                          LAE00580
      X5 = XKOORD(I)                                                   LAE00590
      Y5 = YKOORD(I)                                                   LAE00600
      Z5 = ZKOORD(I)                                                   LAE00610
C                                                                      LAE00620
C*********************************************************************LAE00630
                  DO 20 J=1,MOZAHL                                     LAE00640
                    SPECJ = SPEC(J)                                    LAE00650
              IF (SPECJ.EQ.2) THEN                                     LAE00660
C                                                                      LAE00670
      X6 = XKOORD(J)                                                   LAE00680
      Y6 = YKOORD(J)                                                   LAE00690
      Z6 = ZKOORD(J)                                                   LAE00700
      ALP=ALPHA(J)                                                     LAE00730
      BET=BETA(J)                                                      LAE00740
      GAM=GAMMA(J)                                                     LAE00750
C                                                                      LAE00760
      SINALP=SIN(ALP)                                                  LAE00770
      COSALP=COS(ALP)                                                  LAE00780
      SINBET=SIN(BET)                                                  LAE00790
      COSBET=COS(BET)                                                  LAE00800
      SINGAM=SIN(GAM)                                                  LAE00810
      COSGAM=COS(GAM)                                                  LAE00820
C                                                                      LAE00830
      A11=COSBET*COSGAM                                                LAE00840
      A12=-COSBET*SINGAM                                               LAE00850
      A13=SINBET                                                       LAE00860
```

```
      A21=COSALP*SINGAM+SINALP*SINBET*COSGAM                          LAE00870
      A22=COSALP*COSGAM-SINALP*SINBET*SINGAM                          LAE00880
      A23=-SINALP*COSBET                                              LAE00890
      A31=SINALP*SINGAM-COSALP*SINBET*COSGAM                          LAE00900
      A32=SINALP*COSGAM+COSALP*SINBET*SINGAM                          LAE00910
      A33=COSALP*COSBET                                               LAE00920
C                                                                     LAE00930
      R56 = SQRT((X6-X5)**2+(Y6-Y5)**2+(Z6-Z5)**2)                    LAE00940
      IF (R56.GE.MINDIS.AND.R56.LE.MAXDIS) THEN                       LAE00950
C                                                                     LAE00960
C########CALCULATE COORDINATE OF AMMONIA MOLECULE##########           LAE00970
C                                                                     LAE00980
C ** SPECI = LI  ; SPECJ = NH3**                                      LAE00990
      H3XA=A21*YH1AM+A31*ZHAM + X6                                    LAE01000
      H3YA=A22*YH1AM+A32*ZHAM + Y6                                    LAE01010
      H3ZA=A23*YH1AM+A33*ZHAM + Z6                                    LAE01020
      H4XA=A21*YH2AM+A31*ZHAM + X6                                    LAE01030
      H4YA=A22*YH2AM+A32*ZHAM + Y6                                    LAE01040
      H4ZA=A23*YH2AM+A33*ZHAM + Z6                                    LAE01050
      M8XA=A11*XMAM+A31*ZMAM + X6                                     LAE01060
      M8YA=A12*XMAM+A32*ZMAM + Y6                                     LAE01070
      M8ZA=A13*XMAM+A33*ZMAM + Z6                                     LAE01080
      M10XA=A11*XCAM+A31*ZCAM + X6                                    LAE01090
      M10YA=A12*XCAM+A32*ZCAM + Y6                                    LAE01100
      M10ZA=A13*XCAM+A33*ZCAM + Z6                                    LAE01110
C                                                                     LAE01120
C########CALCULATE DISTANCE BETWEEN LITHIUM AND AMMONIA#########      LAE01130
C                                                                     LAE01140
      XREL1 = H3XA-X5                                                 LAE01150
      YREL1 = H3YA-Y5                                                 LAE01160
      ZREL1 = H3ZA-Z5                                                 LAE01170
      XREL2 = H4XA-X5                                                 LAE01180
      YREL2 = H4YA-Y5                                                 LAE01190
      ZREL2 = H4ZA-Z5                                                 LAE01200
      XREL3 = M8XA-X5                                                 LAE01210
      YREL3 = M8YA-Y5                                                 LAE01220
      ZREL3 = M8ZA-Z5                                                 LAE01230
C *** CALC. OF THE DISTANCEES ***                                     LAE01240
      RH1 = SQRT(XREL1**2+YREL1**2+ZREL1**2)*ANGALU                   LAE01250
      RH2 = SQRT(XREL2**2+YREL2**2+ZREL2**2)*ANGALU                   LAE01260
      RH3 = SQRT(XREL3**2+YREL3**2+ZREL3**2)*ANGALU                   LAE01270
```

```
C     ********************                                          LAE01310
C     LITHIUM-AMMONIA-POT                                          LAE01320
C     ********************                                          LAE01330
      E=0.0                                                        LAE01340
      E1=-(-43772.16987)/(R56*ANGALU)**6+10717.0*EXP(-453.0*R56*ANGALU) LAE01350
     +   +1025.571898*(-0.74207)*(1.0) / (R56*ANGALU)              LAE01360
      E2=-(-31164.80898)/RH1**6-54.76518247*EXP(-0.5763549897*RH1) LAE01370
     +   +1025.571898*(0.24736)*(1.0) / RH1                        LAE01380
     +   +31164.80898/RH2**6-54.76518247*EXP(-0.5763549897*RH2)    LAE01390
     +   +1025.571898*(0.24736)*(1.0) / RH2                        LAE01400
     +   +31164.80898/RH3**6-54.76518247*EXP(-0.5763549897*RH3)    LAE01410
     +   +1025.571898*(0.24736)*(1.0) / RH3                        LAE01420
      E =   E1+E2                                                  LAE01430
C*********************************************************************
        KE=E*2+81                                                  LAE01460
         IENER(KE)=IENER(KE)+1                                     LAE01480
      ENDIF                                                        LAE01500
          ENDIF                                                    LAE01510
C                                                                  LAE01520
 20               CONTINUE                                         LAE01530
 10   CONTINUE                                                     LAE01540
C                                                                  LAE01550
      IF (NSET.EQ.MAX) GOTO 200                                    LAE01560
      GOTO 100                                                     LAE01570
C                                                                  LAE01580
 222   CONTINUE                                                    LAE01590
C                                                                  LAE01600
 200   DO 33 M=1,201                                               LAE01610
       A(M)=(M-101.0)/2.0                                         LAE01620
       TOTAL=TOTAL+IENER(M)                                       LAE01630
 33    CONTINUE                                                    LAE01640
       WRITE(*,*) 'TOTAL=',TOTAL                                  LAE01660
       DO 35 M=1,101                                              LAE01670
       IF(IENER(M).GT.0) PDIST(M)=IENER(M)/TOTAL                  LAE01680
 35    CONTINUE                                                    LAE01700
       WRITE(9,'(9X,I5)')'NSET=',NSET                             LAE01720
       WRITE(9,'(9X,F10.5)')'TOTAL=',TOTAL                        LAE01730
       WRITE(9,*)'      A(M)          PDIST(M)'                   LAE01740
       WRITE(9,'(1X,F10.2,5X,F12.5)') ( A(M),PDIST(M),M=1,101)    LAE01750
       STOP 'FINISHED'                                            LAE01770
       END                                                        LAE01780
```

APPENDIX VIII: PROGRAM DISTRIBUTION OF DISTANCES AND ANGLES FOR TWO AMMONIA MOLECULES IN THE FIRST SHELL OF LITHIUM ION

```
C PROGRAM COS2AM                                                        COS00010
C ***************************************************************      COS00030
C THIS PROGRAM CALCULATES THE DISTRIBUTIONS OF DISTANCES AND            COS00040
C AND ANGLES FOR TWO AMMONIA MOLECULES IN THE FIRST SHELL OF Li(I)      COS00050
C ***************************************************************      COS00060
      INTEGER MOZAHL,NSET,MAX,ICOSW,KCOSW,TOTCOS,NN,DIST,TOTDIS         COS00080
      PARAMETER (MOZAHL = 202)                                          COS00090
      PARAMETER (ICOSW = 201)                                           COS00100
      INTEGER SPEC(MOZAHL),SPECI,SPECJ,ICOS(ICOSW),IDIST(181)           COS00110
      REAL ABSA,ABSB,R56,COSW,VECAB,A(201),PCOS(201),PDIST(181)         COS00120
      REAL AUFLOE,MAXDIS,MINDIS,B(181)                                  COS00130
      PARAMETER (AUFLOE=0.05)                                           COS00140
      REAL   XKOORD (MOZAHL),                                           COS00150
     +       YKOORD (MOZAHL),                                           COS00160
     +       ZKOORD (MOZAHL),                                           COS00170
     +       ALPHA (MOZAHL),                                            COS00180
     +       BETA  (MOZAHL),                                            COS00190
     +       GAMMA (MOZAHL)                                             COS00200
      REAL ALP,BET,GAM,H1X,H1Y,H1Z,H2X,H2Y,H2Z,H7X,H7Y,H7Z,X5,Y5,Z5,    COS00210
     +XAM,YAM,ZAM,X6,Y6,Z6,H3X,H3Y,H3Z,H4X,H4Y,H4Z,H8X,H8Y,H8Z          COS00220
      REAL SINALP,SINBET,SINGAM,COSALP,COSBET,COSGAM,D,                 COS00230
     +          A11,A12,A13,A21,A22,A23,A31,A32,A33                     COS00240
      REAL X3,Y3,Z3                                                     COS00250
      CHARACTER LINE1*80,LINE2*80                                       COS00260
      DATA MINDIS,MAXDIS/0.0,3.8/                                       COS00270
      MAX = 144                                                         COS00280
      D=3.80                                                            COS00290
      OPEN(11,FILE='SAM')                                               COS00300
      OPEN(9,FILE='COSOUT')                                             COS00310
      OPEN(12,FILE='DIST')                                              COS00320
      NSET=0                                                            COS00330
      TOTCOS=0                                                          COS00340
      TOTDIS=0                                                          COS00350
      DO 11 K=1,201                                                     COS00360
           PCOS(K)=0.0                                                  COS00370
           ICOS(K)=0                                                    COS00380
      DO 12 J=1,181                                                     COS00390
```

```
            PDIST(J)=0.0                                                    COS00400
            IDIST(J)=0                                                      COS00410
 12     CONTINUE                                                           COS00420
 11     CONTINUE                                                           COS00430
C ***************************************************************************COS00440
C      WRITE(*,*) 'HAVE YOU ALREADY CHECKED THE MAX-DISTANCE ?'            COS00460
 100    CONTINUE                                                           COS00480
        READ(11,'(A)') LINE1                                               COS00490
        READ(11,'(A)') LINE2                                               COS00500
        READ(11,'(5X,I5,6F10.5)',END=222) (SPEC(I),XKOORD(I),YKOORD(I),    COS00510
       +       ZKOORD(I),ALPHA(I),BETA(I),GAMMA(I),I=1,MOZAHL)             COS00520
        NSET = NSET+1                                                      COS00530
        DO 10 I=1,MOZAHL                                                   COS00540
        SPECI = SPEC(I)                                                    COS00550
        IF (SPECI.NE.3) GOTO 10                                            COS00560
        X5 = XKOORD(I)                                                     COS00570
        Y5 = YKOORD(I)                                                     COS00580
        Z5 = ZKOORD(I)                                                     COS00590
        KCOS = 0                                                           COS00610
        DIST = 0                                                           COS00620
        NN = 0                                                             COS00630
            DO 20 J=1,MOZAHL                                               COS00640
C **********DIPOLE  VECTOR********                                         COS00660
            SPECJ = SPEC(J)                                                COS00670
              IF (SPECJ.EQ.2) THEN                                         COS00680
               X3 = XKOORD(J)                                              COS00700
               Y3 = YKOORD(J)                                              COS00710
               Z3 = ZKOORD(J)                                              COS00720
        R56 = SQRT((X3-X5)**2+(Y3-Y5)**2+(Z3-Z5)**2)                       COS00760
        IF (R56.LE.D) NN=NN+1                                              COS00780
        IF (NN.EQ.1) THEN                                                  COS00800
               X6 = XKOORD(J)                                              COS00810
               Y6 = YKOORD(J)                                              COS00820
               Z6 = ZKOORD(J)                                              COS00830
        ENDIF                                                              COS00840
        IF (NN.EQ.2) THEN                                                  COS00900
               X7 = XKOORD(J)                                              COS00910
               Y7 = YKOORD(J)                                              COS00920
               Z7 = ZKOORD(J)                                              COS00930
        R67 = SQRT((X6-X7)**2+(Y6-Y7)**2+(Z6-Z7)**2)                       COS00940
        VECAB = (X5-X6)*(X7-X6)                                            COS00960
```

```
     +       +(Y5-Y6)*(Y7-Y6)                                          COS00970
     +       +(Z5-Z6)*(Z7-Z6)                                          COS00980
      ABSA = SQRT((X5-X6)**2+(Y5-Y6)**2+(Z5-Z6)**2)                    COS00990
      ABSB = SQRT((X5-X7)**2+(Y5-Y7)**2+(Z5-Z7)**2)                    COS01010
      COSW = VECAB/(ABSA*R67)                                          COS01030
      KCOSW = COSW*100+101                                             COS01040
      ICOS(KCOSW) = ICOS(KCOSW)+1                                      COS01050
      DIST=R67*20-19                                                   COS01060
      IDIST(DIST)=IDIST(DIST)+1                                        COS01070
      GOTO 17                                                          COS01090
            ENDIF                                                      COS01100
       ENDIF                                                           COS01110
20                CONTINUE                                             COS01120
10    CONTINUE                                                         COS01130
17    CONTINUE                                                         COS01140
      IF (NSET.EQ.MAX) GOTO 200                                        COS01160
      GOTO 100                                                         COS01170
222    CONTINUE                                                        COS01190
200    DO 33 M=1,201                                                   COS01210
       A(M) =(M-101)/100.0                                             COS01220
       TOTCOS=TOTCOS+ICOS(M)                                           COS01230
33     CONTINUE                                                        COS01240
       DO 44 N=1,181                                                   COS01250
       B(N)=(N+19.0)/20.0                                              COS01260
       TOTDIS=TOTDIS+IDIST(N)                                          COS01270
44     CONTINUE                                                        COS01280
       WRITE(*,*) TOTCOS                                               COS01290
       DO 35 M=1,201                                                   COS01300
       IF (ICOS(M).GT.0) PCOS(M)=REAL(ICOS(M)/REAL(TOTCOS))            COS01310
35     CONTINUE                                                        COS01320
       DO 36 M=1,181                                                   COS01330
       IF (IDIST(M).GT.0) PDIST(M)=REAL(IDIST(M)/REAL(TOTDIS))         COS01340
36     CONTINUE                                                        COS01350
      WRITE(9,'(9X,I5)')'NSET=',NSET                                   COS01380
      WRITE(9,*)'    A(M)        PCOSW(M)      ICOS(M)'               COS01390
      WRITE(9,'(1X,F8.2,5X,F9.4,3X,I8)')(A(M),PCOS(M),ICOS(M),M=1,201) COS01400
      WRITE(12,*)'    B(M)        PDIST(M)      IDIST(M)'              COS01410
      WRITE(12,'(1X,F8.2,5X,F9.4,3X,I8)')(B(M),PDIST(M),               COS01420
     +                          IDIST(M),M=1,181)                     COS01430
      STOP 'FINISHED'                                                  COS01450
      END                                                              COS01460
```

V I T A

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Two publications have come out of my Master's degree work. They are " The Intermolecular Potential Function for Ammonia-Lithium Ion Based on Ab-initio Calculations " published in Z.Naturforsch.,42a, 143-146,1988, and " A Monte Carlo Study on Preferential Solvation of Lithium Ion in Aqueous Ammonia " in J.Chem.Soc.Faraday.Tran II., forthcoming. During the study towards the Master's degree of Science, I was supported by the **University Development Commission Scholarship.**