

# The Supporting Information

## The CO–Ne van der Waals complex: *ab initio* intermolecular potential energy, interaction induced electric dipole moment and polarizability surfaces, and second virial coefficients

Angelika Baranowska, Berta Fernández

*Department of Physical Chemistry, Faculty of Chemistry,*

*University of Santiago de Compostela,*

*E-15782 Santiago de Compostela, Spain*

Antonio Rizzo

*Istituto per i Processi Chimico-Fisici del Consiglio Nazionale delle Ricerche,*

*Area della Ricerca, via G. Moruzzi 1,*

*loc. S. Cataldo, I-56124 Pisa, Italy*

Branislav Jansik

*Teoretisk Kemi, Kemisk Institut,*

*Aarhus Universitet,*

*Langelandsgade 140,*

*8000 Aarhus C, Denmark*

TABLE I: CO–Ne interaction dipole moment basis set convergence study.  $R$  values in Å,  $\theta$  in  $^\circ$ , and interaction dipole moment values in au.

	$\Delta\mu_{x'} \times 10^3$		$\Delta\mu_{z'} \times 10^3$	
	aug-cc-pVXZ-33211	d-aug-cc-pVXZ-33211	aug-cc-pVXZ-3 3211	d-aug-cc-pVXZ-33211
	$R=3.355, \theta=92.2$			
$X=T$	0.7356	0.7463	5.3578	5.4894
$X=Q$	0.7852	0.7963	5.4661	5.5112
	$R=3.000, \theta=92.2$			
$X=T$	1.4686	1.4816	11.8006	11.9358
$X=Q$	1.5206	1.5382	11.8386	11.8847
	$R=6.000, \theta=92.2$			
$X=T$	-0.0089	-0.0118	0.3296	0.3319
$X=Q$	-0.0023	-0.0026	0.3234	0.3265

TABLE II: CO–Ne static electric dipole polarizability and Cauchy moment basis set selection  $R$  values in Å,  $\theta$  in  $^\circ$ , and the static electric dipole polarizability and Cauchy moment values in au.

	$\Delta\alpha_{ave}(R, \theta) \times 10^2$		$\Delta S(-4)_{ave}(R, \theta) \times 10^2$	
	aug-cc-pVXZ-33211	d-aug-cc-pVXZ-33211	aug-cc-pVXZ-33211	d-aug-cc-pVXZ-33211
	$R=3.355, \theta=92.2$			
$X=T$	-3.932	-4.322	-28.713	-31.450
$X=Q$	-4.093	-4.169	-29.033	-29.933
	$R=3.000, \theta=92.2$			
$X=T$	-8.681	-9.103	-60.823	-63.797
$X=Q$	-8.777	-8.841	-60.439	-61.311
	$R=6.000, \theta=92.2$			
$X=T$	-0.248	-0.345	0.590	-0.083
$X=Q$	-0.319	-0.349	0.200	-0.103

TABLE III: CO–Ne interaction induced energies evaluated with the CCSD(T) method and the d-aug-cc-pVTZ-33211 basis set.  $R$  values in Å,  $\theta$  in  $^\circ$ , and energy values in  $\text{cm}^{-1}$ . See the text for details.

R [Å]	$\theta$ [ $^\circ$ ]									
	0.0	20.0	40.0	60.0	80.0	100.0	120.0	140.0	160.0	180.0
2.20	16310.670	13632.070	8562.292	4848.532	3216.475	3431.050	6464.548	15138.227	30415.861	40265.513
2.30	10596.381	8870.258	5567.400	3131.142	2073.783	2283.404	4542.406	10978.372	22099.189	29018.710
2.50	4369.925	3655.624	2270.940	1243.529	810.645	959.730	2159.249	5559.085	11248.976	14624.553
2.75	1346.903	1114.329	661.459	328.135	194.609	269.411	776.207	2220.090	4579.481	5932.341
3.00	348.729	276.360	137.092	37.888	1.203	32.038	229.210	808.003	1749.471	2279.964
3.15	122.679	88.213	23.198	-21.054	-36.184	-20.032	86.138	410.255	941.882	1240.453
3.25	43.563	23.152	-14.452	-38.686	-46.306	-36.579	31.464	248.014	607.421	809.462
3.40	-16.771	-25.371	-40.165	-48.095	-49.929	-46.305	-13.955	100.331	296.023	406.785
3.50	-34.626	-39.000	-45.776	-48.181	-48.217	-47.011	-28.925	43.342	171.446	244.630
3.60	-42.589	-44.423	-46.487	-45.791	-44.919	-45.249	-36.462	7.479	89.639	137.277
3.75	-44.448	-44.315	-42.890	-40.116	-38.767	-40.330	-39.472	-21.172	18.679	42.691
3.85	-42.282	-41.538	-39.128	-35.910	-34.538	-36.476	-38.382	-29.916	-6.804	7.763
4.00	-37.006	-35.890	-33.026	-29.823	-28.594	-30.709	-34.609	-34.397	-26.080	-20.006
4.10	-33.062	-31.909	-29.110	-26.142	-25.053	-27.133	-31.507	-34.089	-31.292	-28.466
4.25	-27.323	-26.278	-23.825	-21.333	-20.457	-22.363	-26.768	-31.246	-32.910	-32.793
4.35	-23.841	-22.923	-20.766	-18.604	-17.856	-19.607	-23.788	-28.636	-31.692	-32.468
4.50	-19.296	-18.586	-16.870	-15.161	-14.576	-16.078	-19.770	-24.501	-28.315	-29.639
5.00	-9.666	-9.354	-8.599	-7.830	-7.589	-8.399	-10.428	-13.319	-16.047	-17.111
6.00	-2.858	-2.765	-2.577	-2.410	-2.391	-2.620	-3.125	-3.806	-4.431	-4.694
7.00	-1.041	-1.017	-0.963	-0.915	-0.912	-0.987	-1.139	-1.334	-1.501	-1.567
10.00	-0.113	-0.112	-0.107	-0.103	-0.102	-0.108	-0.119	-0.134	-0.145	-0.150
15.00	-0.010	-0.010	-0.009	-0.009	-0.009	-0.009	-0.010	-0.011	-0.011	-0.012
20.00	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002	-0.002

TABLE IV: CO–Ne interaction induced dipole moment  $x'$ -components evaluated with the CCSD method and the d-aug-cc-pVTZ-33211 basis set.  $R$  values in Å,  $\theta$  in  $^\circ$ , and dipole moment values in au. See the text for details.

R [Å]	$\Delta\mu_{x'} \times 10^3$									
	$\theta [^\circ]$									
	0.0	20.0	40.0	60.0	80.0	100.0	120.0	140.0	160.0	180.0
2.20	76.2747	86.0037	80.4026	52.0204	24.1674	-9.1132	-82.2045	-224.4778	-383.6192	-438.3663
2.30	54.2913	60.9372	58.2968	39.4547	19.3860	-7.0190	-65.9174	-178.1162	-302.8602	-349.9192
2.50	26.1321	29.9714	30.7074	22.9491	12.5490	-4.3229	-42.4944	-111.5896	-186.3854	-216.5582
2.75	8.5632	11.0759	13.5003	11.8729	7.3947	-2.5078	-24.5739	-61.2292	-98.6981	-113.9273
3.00	0.9812	2.8524	5.6368	6.3293	4.4788	-1.5500	-14.2530	-32.7316	-49.5985	-56.0839
3.15	-1.1126	0.4913	3.2018	4.4409	3.3783	-1.2002	-10.3331	-22.1474	-31.5882	-34.8612
3.25	-1.9162	-0.4627	2.1388	3.5522	2.8257	-1.0273	-8.3732	-16.9567	-22.8621	-24.6019
3.40	-2.5496	-1.2918	1.0990	2.6003	2.1943	-0.8323	-6.1624	-11.2431	-13.4165	-13.5501
3.50	-2.7176	-1.5743	0.6609	2.1481	1.8731	-0.7342	-5.0616	-8.4896	-8.9714	-8.3906
3.60	-2.7547	-1.7151	0.3615	1.7997	1.6119	-0.6550	-4.1884	-6.3748	-5.6430	-4.5634
3.75	-2.6577	-1.7559	0.0884	1.4169	1.3055	-0.5622	-3.2031	-4.1059	-2.2213	-0.6956
3.85	-2.5346	-1.7139	-0.0158	1.2284	1.1445	-0.5133	-2.7097	-3.0422	-0.7149	0.9615
4.00	-2.3105	-1.5968	-0.1003	1.0137	0.9507	-0.4536	-2.1464	-1.9223	0.7357	2.4896
4.10	-2.1519	-1.5005	-0.1261	0.9035	0.8461	-0.4207	-1.8594	-1.4073	1.3165	3.0545
4.25	-1.9167	-1.3475	-0.1377	0.7726	0.7170	-0.3789	-1.5246	-0.8745	1.8016	3.4538
4.35	-1.7671	-1.2460	-0.1346	0.7024	0.6457	-0.3549	-1.3497	-0.6339	1.9485	3.5187
4.50	-1.5582	-1.1008	-0.1214	0.6158	0.5560	-0.3235	-1.1404	-0.3895	2.0021	3.4317
5.00	-1.0152	-0.7125	-0.0596	0.4245	0.3549	-0.2444	-0.7163	-0.0843	1.5907	2.5566
6.00	-0.4597	-0.3119	0.0058	0.2293	0.1648	-0.1465	-0.3535	-0.0267	0.7412	1.1679
7.00	-0.2431	-0.1618	0.0119	0.1292	0.0832	-0.0908	-0.1930	-0.0119	0.3802	0.5922
10.00	-0.0557	-0.0356	0.0066	0.0322	0.0157	-0.0277	-0.0463	0.0015	0.0897	0.1351
15.00	-0.0094	-0.0055	0.0024	0.0064	0.0019	-0.0069	-0.0093	0.0014	0.0187	0.0272
20.00	-0.0024	-0.0012	0.0011	0.0020	0.0002	-0.0026	-0.0030	0.0008	0.0064	0.0091

TABLE V: CO–Ne interaction induced dipole moment  $z'$ -components evaluated with the CCSD method and the d-aug-cc-pVTZ-33211 basis set.  $R$  values in Å,  $\theta$  in  $^\circ$ , and dipole moment values in au. See the text for details.

R [Å]	$\Delta\mu_{z'} \times 10^3$									
	$\theta [^\circ]$									
	0.0	20.0	40.0	60.0	80.0	100.0	120.0	140.0	160.0	180.0
2.20	0.0000	13.8170	31.4129	38.3048	51.1240	101.8488	207.7941	329.8573	313.7426	0.0000
2.30	0.0000	8.2895	21.1519	28.4136	40.5000	80.3836	159.9171	246.2609	223.9393	0.0000
2.50	0.0000	2.1096	8.9521	15.4285	25.3313	49.9326	93.9762	136.0140	115.1970	0.0000
2.75	0.0000	-0.9995	1.9763	6.7893	13.9778	27.4108	47.5586	63.3244	49.9824	0.0000
3.00	0.0000	-1.9394	-0.7851	2.6164	7.7082	15.0692	23.5141	27.9572	20.3211	0.0000
3.15	0.0000	-2.0533	-1.4725	1.2883	5.4347	10.5898	15.1965	16.3007	10.9269	0.0000
3.25	0.0000	-2.0351	-1.7055	0.7061	4.3334	8.4120	11.2806	10.9849	6.7387	0.0000
3.40	0.0000	-1.9284	-1.8428	0.1421	3.1293	6.0193	7.1269	5.5420	2.5506	0.0000
3.50	0.0000	-1.8274	-1.8426	-0.0885	2.5490	4.8592	5.1979	3.1259	0.7468	0.0000
3.60	0.0000	-1.7150	-1.7967	-0.2388	2.0998	3.9570	3.7574	1.4011	-0.5013	0.0000
3.75	0.0000	-1.5398	-1.6777	-0.3611	1.6070	2.9622	2.2625	-0.2616	-1.6388	0.0000
3.85	0.0000	-1.4252	-1.5808	-0.3967	1.3666	2.4750	1.5854	-0.9361	-2.0567	0.0000
4.00	0.0000	-1.2628	-1.4270	-0.4082	1.0980	1.9298	0.8958	-1.5189	-2.3532	0.0000
4.10	0.0000	-1.1628	-1.3248	-0.3983	0.9636	1.6572	0.5897	-1.7124	-2.4041	0.0000
4.25	0.0000	-1.0259	-1.1782	-0.3691	0.8090	1.3447	0.2846	-1.8185	-2.3478	0.0000
4.35	0.0000	-0.9434	-1.0868	-0.3445	0.7292	1.1842	0.1529	-1.8100	-2.2563	0.0000
4.50	0.0000	-0.8319	-0.9607	-0.3048	0.6342	0.9950	0.0262	-1.7285	-2.0778	0.0000
5.00	0.0000	-0.5524	-0.6350	-0.1842	0.4390	0.6220	-0.0992	-1.2703	-1.4366	0.0000
6.00	0.0000	-0.2647	-0.2951	-0.0588	0.2471	0.3071	-0.0671	-0.6045	-0.6532	0.0000
7.00	0.0000	-0.1433	-0.1562	-0.0218	0.1436	0.1636	-0.0463	-0.3219	-0.3353	0.0000
10.00	0.0000	-0.0339	-0.0348	0.0003	0.0384	0.0359	-0.0189	-0.0796	-0.0767	0.0000
15.00	0.0000	-0.0061	-0.0055	0.0018	0.0086	0.0064	-0.0056	-0.0169	-0.0153	0.0000
20.00	0.0000	-0.0017	-0.0013	0.0011	0.0030	0.0018	-0.0023	-0.0058	-0.0051	0.0000

TABLE VI: CO–Ne static interaction induced dipole polarizability evaluated with the CCSD method and the d-aug-cc-pVTZ-33211 basis set.  $R$  values in Å,  $\theta$  in  $^\circ$ , and polarizability values in au. See the text for details.

R [Å]	$\Delta\alpha(R, \theta) \times 10^3$									
	$\theta [^\circ]$									
	0.0	20.0	40.0	60.0	80.0	100.0	120.0	140.0	160.0	180.0
2.20	-115.4613	-98.3988	-147.0608	-260.9449	-341.4797	-327.7186	-161.7697	335.0151	1501.5630	2515.3060
2.30	-145.9609	-132.5362	-160.4494	-240.1714	-301.3699	-299.0246	-201.2248	88.3362	689.1333	1129.3098
2.50	-128.5488	-121.5218	-135.3135	-181.8640	-221.9057	-231.9219	-215.4974	-163.8601	-71.8917	-23.2417
2.75	-65.5073	-64.8912	-78.8583	-112.1496	-140.6216	-153.2192	-172.5509	-227.9482	-316.5348	-370.2214
3.00	-11.6671	-15.4014	-32.9328	-62.2806	-84.8397	-93.8324	-114.4937	-183.8708	-294.2215	-355.4088
3.15	10.1085	4.7815	-14.1943	-42.0646	-62.0173	-68.1440	-83.6366	-144.3420	-243.2479	-297.3384
3.25	20.4391	14.4171	-5.0613	-31.9308	-50.3384	-54.6478	-66.0662	-118.5230	-206.3623	-254.3504
3.40	30.7007	24.0852	4.4947	-20.7326	-37.0320	-38.9716	-44.4822	-83.8162	-153.8404	-192.3972
3.50	34.7433	27.9699	8.6594	-15.3808	-30.3982	-31.0473	-33.1000	-64.1701	-122.7933	-155.4235
3.60	37.0733	30.2863	11.4708	-11.3320	-25.1615	-24.7584	-23.8695	-47.4826	-95.6493	-122.8709
3.75	38.2040	31.5920	13.8010	-7.1090	-19.3290	-17.7618	-13.4644	-27.7170	-62.4110	-82.6599
3.85	37.8463	31.4396	14.4496	-5.2093	-16.4677	-14.3655	-8.4236	-17.6781	-44.9333	-61.3106
4.00	36.2555	30.2352	14.5301	-3.3166	-13.2891	-10.6776	-3.0758	-6.5434	-24.8218	-36.4786
4.10	34.7574	29.0237	14.1902	-2.5108	-11.7225	-8.9276	-0.6652	-1.2701	-14.8637	-24.0201
4.25	32.1816	26.8929	13.3399	-1.7563	-9.9565	-7.0599	1.6787	4.1517	-4.0507	-10.2744
4.35	30.3786	25.3848	12.6485	-1.4591	-9.0626	-6.1837	2.6109	6.4809	0.9670	-3.7585
4.50	27.6976	23.1298	11.5437	-1.2043	-8.0151	-5.2485	3.3575	8.5792	6.0320	3.0085
5.00	20.0310	16.6584	8.1913	-1.0069	-5.8719	-3.7702	3.1627	9.2606	10.9815	10.6755
6.00	11.0773	9.1448	4.3349	-0.8526	-3.6335	-2.5976	1.2527	5.2381	7.4007	7.9210
7.00	6.6883	5.4939	2.5261	-0.6713	-2.4175	-1.8795	0.3823	2.8701	4.4081	4.8588
10.00	2.1252	1.7328	0.7570	-0.2982	-0.8965	-0.7710	-0.0665	0.7937	1.4176	1.6341
15.00	0.6051	0.4936	0.2161	-0.0866	-0.2647	-0.2400	-0.0424	0.2198	0.4282	0.5057
20.00	0.2504	0.2045	0.0902	-0.0353	-0.1108	-0.1029	-0.0214	0.0912	0.1836	0.2188

TABLE VII: CO–Ne interaction Cauchy moments evaluated with the CCSD method and the d-aug-cc-pVTZ-33211 basis set.  $R$  values in Å,  $\theta$  in  $^\circ$ , and polarizability values in au. See the text for details.

R [Å]	$\Delta S(-4)_{ave}(R, \theta) \times 10^2$									
	$\theta [^\circ]$									
	0.0	20.0	40.0	60.0	80.0	100.0	120.0	140.0	160.0	180.0
2.20	169.5300	130.9434	34.6874	-58.3727	-122.3038	-125.3054	66.3545	910.5359	3641.0731	6709.6567
2.30	91.3709	61.8702	-7.1688	-75.0179	-124.0725	-136.0503	-20.7663	510.3739	1976.9556	3310.4195
2.50	19.6256	1.2738	-39.9232	-80.6894	-111.5788	-131.3212	-108.1808	72.2072	509.1612	817.8278
2.75	-2.5778	-13.9650	-39.8852	-65.6203	-84.3496	-102.5450	-124.8680	-121.8402	-66.0034	-26.7323
3.00	0.0054	-8.0954	-27.0417	-45.8153	-57.6643	-69.5831	-99.6809	-150.8589	-200.5026	-222.5346
3.15	4.4218	-2.5541	-19.0609	-35.3066	-44.3836	-52.2766	-79.3052	-137.1824	-204.8735	-237.0573
3.25	7.3184	0.9009	-14.3585	-29.2759	-36.8828	-42.3163	-65.9913	-123.0114	-193.9842	-228.3066
3.40	10.9782	5.2236	-8.5046	-21.7601	-27.5936	-29.8529	-47.8682	-99.3444	-167.9953	-201.8068
3.50	12.8236	7.4367	-5.4154	-17.7120	-22.5953	-23.1203	-37.4161	-83.7743	-148.1475	-180.2087
3.60	14.1777	9.1212	-2.9297	-14.3520	-18.4369	-17.5321	-28.3858	-69.2330	-128.2430	-157.9663
3.75	15.3689	10.7616	-0.1858	-10.4200	-13.5434	-11.0231	-17.4361	-50.1414	-100.3537	-126.0937
3.85	15.6882	11.3581	1.0956	-8.4153	-11.0288	-7.7434	-11.7269	-39.4300	-83.8252	-106.8622
4.00	15.6182	11.6773	2.3769	-6.1401	-8.1469	-4.1018	-5.2170	-26.3451	-62.6342	-81.8231
4.10	15.2966	11.5993	2.8987	-5.0122	-6.7011	-2.3613	-2.0350	-19.4521	-50.9125	-67.7621
4.25	14.5375	11.1828	3.3201	-3.7608	-5.0749	-0.5356	1.3539	-11.4787	-36.6626	-50.4121
4.35	13.9118	10.7706	3.4255	-3.1518	-4.2706	0.2785	2.8776	-7.4976	-29.1364	-41.1011
4.50	12.8807	10.0374	3.4081	-2.4829	-3.3720	1.0621	4.3366	-3.1238	-20.3297	-30.0218
5.00	9.4663	7.4276	2.7070	-1.4142	-1.8864	1.6495	5.2112	2.8598	-5.3944	-10.3006
6.00	4.9836	3.8866	1.3662	-0.8057	-1.0389	0.8028	2.8362	2.5141	-0.1864	-1.8593
7.00	2.8057	2.1684	0.7065	-0.5492	-0.7023	0.2780	1.3428	1.2101	-0.0671	-0.8504
10.00	0.7560	0.5756	0.1610	-0.1963	-0.2562	-0.0265	0.2253	0.2179	-0.0224	-0.1698
15.00	0.1838	0.1404	0.0405	-0.0472	-0.0677	-0.0223	0.0341	0.0471	0.0187	-0.0010
20.00	0.0689	0.0530	0.0162	-0.0064	-0.0263	-0.0118	0.0073	0.0180	0.0143	0.0104