Electronic Supplementary Information

Structure and C···N tetrel-bonding of the isopropylamine-CO_2 complex studied by microwave spectroscopy and theoretical calculations

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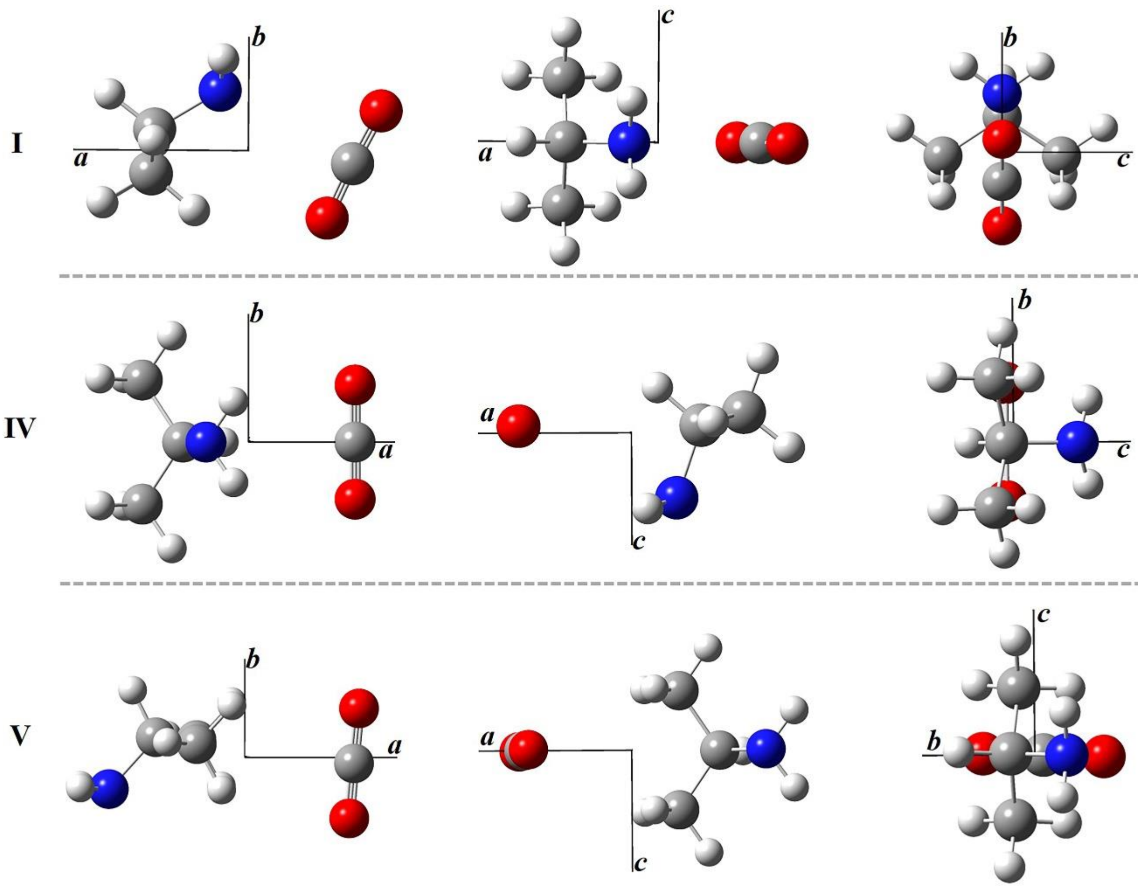

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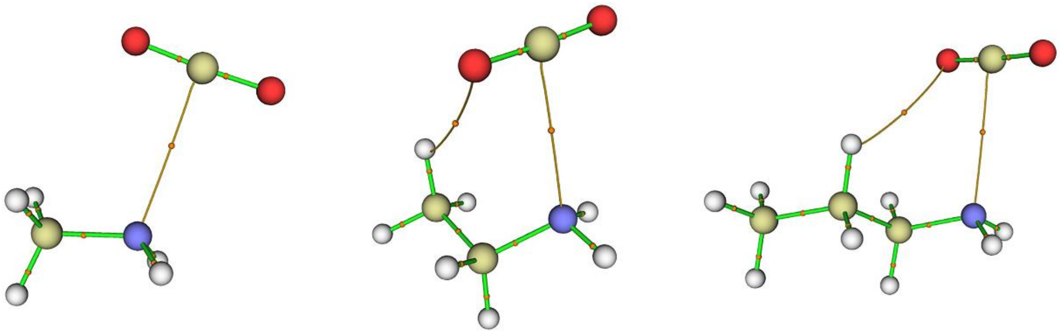

$CO_2 \cdots MA$ $CO_2 \cdots EA$ $CO_2 \cdots NPA$

Fig. S2. QTAIM analyses of the most stable isomers of the complexes of CO_2 with MA, EA and NPA. The BCPs are indicated with orange dots. The bond paths are shown in gold lines.

Table S1. Spectroscopic parameters of the six most stable isomers of CO_2···IPA adduct calculated at ωB97XD/jun-cc-pVTZ level of theory.

Parameters[a]	I	II	III	IV	V	VI
A(MHz)	3881	4804	3879	3781	4368	4357
B(MHz)	1249	1113	1169	1208	1016	1024
C(MHz)	1191	1040	1043	1050	1006	1011
χ_{aa} (MHz)	-1.464	-3.525	-1.766	-2.285	0.790	0.216
(χ_{bb}-χ_{cc}) (MHz)	-2.599	-0.656	3.497	1.879	-4.919	5.243
$\|\mu_a\|$ (D)	1.4	1.7	0.9	0.9	0.8	0.6
$\|\mu_b\|$ (D)	1.0	0.6	0.2	0.0	1.0	0.0
$\|\mu_c\|$ (D)	0.0	0.1	0.8	0.7	0.0	1.0
P_{cc}(uÅ^2)	55.26	36.66	39.03	35.35	55.38	54.82
ΔE_0 (cm^{-1})	0	142	725	795	803	809
$\Delta E_{0,BSSE}$ (cm^{-1})	0	141	717	789	793	799
$\Delta G_{298.15k}$ (cm^{-1})	0	379	823	989	999	859
E_D	13.0	12.3	4.5	3.6	3.6	4.5

[a] A, B, and C are the rotational constants, χ_{aa}, χ_{ac} and χ_{bb}-χ_{cc} are 14N nuclear quadrupole coupling constants, $|\mu_g$, g = a, b, c$|$ are electric dipole moment components, P_{cc} is the planar moment of inertia (= $\Sigma_i m_i c_i^2$), σ is standard deviation of the fit, N is number of transitions in the fit, ΔE_0 and $\Delta E_{0,\,BSSE}$ are the relative energy with zero-point energy (ZPE) and BSSE corrections, ΔG is the relative Gibbs free energy with respect to the most stable isomer calculated at 298.15 K, E_D is the dissociation energies with ZPE and BSSE corrections.

Table S2. Spectroscopic parameters of the six most stable isomers of CO_2···IPA adduct calculated at MP2/6-311++G(2d,p) level of theory.

Parameters[a]	I	II	III	IV	V	VI
A(MHz)	3851	4777	3873	3732	4323	4310
B(MHz)	1257	1133	1176	1215	1021	1025
C(MHz)	1195	1061	1050	1056	1008	1009
χ_{aa} (MHz)	-1.554	-3.595	-1.713	-2.393	0.733	0.187
(χ_{bb}-χ_{cc}) (MHz)	-2.260	-0.307	3.396	1.556	-4.601	5.059
$\|\mu_a\|$ (D)	1.4	1.7	0.9	1.0	0.8	0.7
$\|\mu_b\|$ (D)	0.9	0.5	0.3	0.0	1.2	0.0
$\|\mu_c\|$ (D)	0.0	0.1	0.9	0.8	0.0	1.1
P_{cc}(uÅ^2)	55.19	37.76	39.46	36.39	55.26	54.72
ΔE_0 (cm^{-1})	0	187	688	710	768	930
$\Delta E_{0,BSSE}$ (cm^{-1})	0	188	588	605	616	779
$\Delta G_{298.15k}$ (cm^{-1})	0	183	541	968	531	721
E_D	10.1	10.0	3.0	2.8	2.7	2.9

[a] A, B, and C are the rotational constants, χ_{aa}, χ_{ac} and χ_{bb}-χ_{cc} are 14N nuclear quadrupole coupling constants, $|\mu_g$, g = a, b, c$|$ are electric dipole moment components, P_{cc} is the planar moment of inertia (= $\Sigma_i m_i c_i^2$), σ is standard deviation of the fit, N is number of transitions in the fit, ΔE_0 and $\Delta E_{0,\,BSSE}$ are the relative energy with zero-point energy (ZPE) and BSSE corrections, ΔG is the relative Gibbs free energy with respect to the most stable isomer calculated at 298.15 K, E_D is the dissociation energies with ZPE and BSSE corrections.

Table S3. Spectroscopic parameters of the six most stable isomers of CO_2···IPA adduct calculated at B3LYP-D3(BJ)/jun-cc-pVTZ level of theory.

Parameters[a]	I	II	III	IV	V	VI
A(MHz)	3878	4788	3868	3760	4344	4329
B(MHz)	1265	1127	1170	1208	1018	1021
C(MHz)	1207	1050	1045	1050	1008	1008
χ_{aa} (MHz)	-1.479	-3.563	-1.744	-2.323	0.807	0.215
(χ_{bb}-χ_{cc}) (MHz)	-2.654	-0.689	3.535	1.913	-5.003	5.281
$\|\mu_a\|$ (D)	1.5	1.8	0.8	0.8	0.8	0.5
$\|\mu_b\|$ (D)	1.0	0.6	0.2	0.0	1.1	0.0
$\|\mu_c\|$ (D)	0.0	0.1	0.8	0.7	0.0	1.0
P_{cc}(uÅ^2)	55.56	36.33	39.49	35.73	55.71	55.18
ΔE_0 (cm^{-1})	0	98	717	720	783	964
$\Delta E_{0,BSSE}$ (cm^{-1})	0	99	709	714	772	853
$\Delta G_{298.15k}$ (cm^{-1})	0	27	542	496	647	717
E_D	14.1	14.1	5.6	5.5	4.8	5.1

[a] A, B, and C are the rotational constants, χ_{aa}, χ_{ac} and χ_{bb}-χ_{cc} are 14N nuclear quadrupole coupling constants, $|\mu_{g,}$ g = a, b, c| are electric dipole moment components, P_{cc} is the planar moment of inertia (= $\Sigma_i m_i c_i^2$), σ is standard deviation of the fit, N is number of transitions in the fit, ΔE_0 and $\Delta E_{0,\ BSSE}$ are the relative energy with zero-point energy (ZPE) and BSSE corrections, ΔG is the relative Gibbs free energy with respect to the most stable isomer calculated at 298.15 K, E_D is the dissociation energies with ZPE and BSSE corrections.

Table S4. Spectroscopic parameters of the six most stable isomers of CO_2···IPA adduct calculated at B2PLYP-D3(BJ)/jun-cc-pVTZ level of theory.

Parameters[a]	I	II	III	IV	V	VI
A(MHz)	3874	4788	3875	3757	4342	4323
B(MHz)	1257	1123	1164	1204	1010	1015
C(MHz)	1198	1041	1042	1046	998	1000
χ_{aa} (MHz)	-1.440	-3.503	-1.731	-2.272	0.797	0.195
(χ_{bb}-χ_{cc}) (MHz)	-2.546	-0.600	3.380	1.790	-4.818	5.098
$\lvert\mu_a\rvert$ (D)	1.4	1.7	0.9	0.9	0.8	0.6
$\lvert\mu_b\rvert$ (D)	0.9	0.5	0.2	0.0	1.1	0.0
$\lvert\mu_c\rvert$ (D)	0.0	0.1	0.8	0.7	0.0	1.0
P_{cc}(uÅ^2)	55.33	35.05	39.79	35.56	55.19	54.72
ΔE_0 (cm^{-1})	0	132	683	693	747	858
$\Delta E_{0,BSSE}$ (cm^{-1})	0	134	669	679	717	829
$\Delta G_{298.15k}$ (cm^{-1})	0	34	453	358	503	635
E_D	12.6	12.6	4.6	4.5	4.1	4.3

[a] A, B, and C are the rotational constants, χ_{aa}, χ_{ac} and χ_{bb}-χ_{cc} are 14N nuclear quadrupole coupling constants, $|\mu_{g,}$ g = a, b, c| are electric dipole moment components, P_{cc} is the planar moment of inertia (= $\Sigma_i m_i c_i^2$), σ is standard deviation of the fit, N is number of transitions in the fit, ΔE_0 and $\Delta E_{0,\ BSSE}$ are the relative energy with zero-point energy (ZPE) and BSSE corrections, ΔG is the relative Gibbs free energy with respect to the most stable isomer calculated at 298.15 K, E_D is the dissociation energies with ZPE and BSSE corrections.

Table S5. Experimental transition frequencies of the observed parent species of isomer **I** of CO_2···IPA.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs} (MHz)	$\Delta\nu_{obs\text{-}calc}$ (MHz)
3	0	3	2	2	0	2	1	7244.0735	0.0008
3	0	3	3	2	0	2	2	7244.1268	0.0003
3	0	3	4	2	0	2	3	7244.1548	0.0008
3	1	3	2	2	1	2	1	7166.9553	-0.0032
3	1	3	3	2	1	2	2	7166.8913	-0.0012
3	1	3	4	2	1	2	3	7167.0298	0.0010
3	1	2	2	2	1	1	1	7326.5527	0.0041
3	1	2	3	2	1	1	2	7326.3719	0.0003
3	1	2	4	2	1	1	3	7326.4826	0.0011
3	2	2	2	2	2	1	1	7247.1798	0.0015
3	2	2	3	2	2	1	2	7246.5030	0.0012
3	2	2	4	2	2	1	3	7246.9320	-0.0047
3	2	1	2	2	2	0	1	7250.4239	0.0004
3	2	1	3	2	2	0	2	7249.7611	0.0003
3	2	1	4	2	2	0	3	7250.1799	-0.0045
4	0	4	3	3	0	3	2	9654.8795	-0.0029
4	0	4	4	3	0	3	3	9654.8963	0.0025
4	0	4	5	3	0	3	4	9654.9185	-0.0010
4	1	4	4	3	1	3	3	9554.8124	0.0023
4	1	4	5	3	1	3	4	9554.8779	0.0020
4	1	3	4	3	1	2	3	9767.4044	0.0010
4	1	3	5	3	1	2	4	9767.4537	0.0012
4	1	3	3	3	1	2	2	9767.4637	-0.0041
4	2	3	3	3	2	2	2	9661.6874	0.0010
4	2	3	5	3	2	2	4	9661.6387	0.0002
4	2	3	4	3	2	2	3	9661.4537	0.0015
4	2	2	3	3	2	1	2	9669.8008	0.0022
4	2	2	4	3	2	1	3	9669.5856	0.0034
4	2	2	5	3	2	1	4	9669.7554	0.0024
5	0	5	4	4	0	4	3	12062.3086	-0.0056
5	0	5	5	4	0	4	4	12062.3162	0.0075
5	0	5	6	4	0	4	5	12062.3346	-0.0006
5	1	5	4	4	1	4	3	11941.7629	0.0031
5	1	5	5	4	1	4	4	11941.7515	-0.0018
5	1	5	6	4	1	4	5	11941.7957	0.0026
5	1	4	4	4	1	3	3	12207.4029	-0.0041
5	1	4	5	4	1	3	4	12207.3733	-0.0004
5	1	4	6	4	1	3	5	12207.4029	0.0006
5	2	4	5	4	2	3	4	12075.5280	0.0009
5	2	4	6	4	2	3	5	12075.6260	-0.0005
5	2	4	4	4	2	3	3	12075.6433	0.0066

5	2	3	4	4	2	2	3	12091.8390	0.0056
5	2	3	5	4	2	2	4	12091.7475	0.0021
5	2	3	6	4	2	2	5	12091.8231	-0.0022
5	3	3	4	4	3	2	3	12079.2884	0.0007
5	3	3	5	4	3	2	4	12079.0289	-0.0030
5	3	3	6	4	3	2	5	12079.2350	-0.0020
5	3	2	4	4	3	1	3	12079.4532	-0.0022
5	3	2	5	4	3	1	4	12079.1960	-0.0040
5	3	2	6	4	3	1	5	12079.4015	-0.0033
6	0	6	5	5	0	5	4	14465.6174	0.0110
6	0	6	6	5	0	5	5	14465.5918	0.0005
6	0	6	7	5	0	5	6	14465.6174	-0.0024
6	1	6	5	5	1	5	4	14327.5495	0.0054
6	1	6	6	5	1	5	5	14327.5442	0.0043
6	1	6	7	5	1	5	6	14327.5675	-0.0004
6	1	5	5	5	1	4	4	14646.0392	-0.0016
6	1	5	6	5	1	4	5	14646.0235	0.0046
6	1	5	7	5	1	4	6	14646.0392	0.0002
6	2	5	5	5	2	4	4	14488.6996	0.0007
6	2	5	6	5	2	4	5	14488.6372	-0.0005
6	2	5	7	5	2	4	6	14488.6996	0.0010
6	2	4	5	5	2	3	4	14516.9456	0.0028
6	2	4	6	5	2	3	5	14516.9089	0.0020
6	2	4	7	5	2	3	6	14516.9456	0.0010
6	3	4	5	5	3	3	4	14495.5432	-0.0053
6	3	4	6	5	3	3	5	14495.4092	-0.0014
6	3	4	7	5	3	3	6	14495.5316	0.0019
6	3	3	5	5	3	2	4	14495.9917	-0.0040
6	3	3	6	5	3	2	5	14495.8576	-0.0010
6	3	3	7	5	3	2	6	14495.9776	0.0006
7	0	7	6	6	0	6	5	16864.0545	-0.0052
7	0	7	7	6	0	6	6	16864.0366	-0.0013
7	0	7	8	6	0	6	7	16864.0713	0.0026
7	1	7	6	6	1	6	5	16711.9920	-0.0008
7	1	7	7	6	1	6	6	16711.9920	0.0034
7	1	7	8	6	1	6	7	16712.0049	-0.0055
7	1	6	6	6	1	5	5	17083.0523	-0.0015
7	1	6	8	6	1	5	7	17083.0523	-0.0008
7	2	6	6	6	2	5	5	16900.6648	0.0023
7	2	6	7	6	2	5	6	16900.6237	0.0001
7	2	6	8	6	2	5	7	16900.6648	-0.0002
7	2	5	6	6	2	4	5	16945.5901	0.0058
7	2	5	8	6	2	4	7	16945.5901	0.0013
7	3	5	6	6	3	4	5	16912.0299	0.0012

7	3	5	7	6	3	4	6	16911.9463	-0.0006
7	3	5	8	6	3	4	7	16912.0166	-0.0052
7	3	4	6	6	3	3	5	16913.0358	0.0016
7	3	4	7	6	3	3	6	16912.9534	-0.0003
7	3	4	8	6	3	3	7	16913.0244	-0.0030
8	0	8	7	7	0	7	6	19257.0898	-0.0040
8	0	8	8	7	0	7	7	19257.0630	-0.0040
8	0	8	9	7	0	7	8	19257.1024	0.0021
8	1	8	7	7	1	7	6	19094.9448	0.0044
8	1	8	8	7	1	7	7	19094.9378	0.0022
8	1	8	9	7	1	7	8	19094.9493	-0.0047
8	1	7	7	7	1	6	6	19518.1102	-0.0005
8	1	7	9	7	1	6	8	19518.1102	-0.0001
8	2	7	7	7	2	6	6	19311.3427	0.0059
8	2	7	8	7	2	6	7	19311.3111	0.0016
8	2	7	9	7	2	6	8	19311.3427	0.0027
8	2	6	7	7	2	5	6	19378.1187	0.0084
8	2	6	8	7	2	5	7	19378.1187	0.0038
8	2	6	9	7	2	5	8	19378.1187	0.0033
8	3	6	7	7	3	5	6	19328.6835	-0.0018
8	3	6	8	7	3	5	7	19328.6337	0.0002
8	3	6	9	7	3	5	8	19328.6835	0.0002
8	3	5	7	7	3	4	6	19330.6936	-0.0005
8	3	5	8	7	3	4	7	19330.6488	0.0045
8	3	5	9	7	3	4	8	19330.6936	0.0013
2	2	1	1	1	1	0	0	12745.4507	-0.0029
2	2	1	2	1	1	0	1	12744.7936	0.0032
2	2	1	3	1	1	0	2	12744.8937	0.0023
2	2	0	1	1	1	1	0	12798.3126	-0.0034
2	2	0	2	1	1	1	1	12799.3281	-0.0005
2	2	0	3	1	1	1	2	12798.7596	0.0031
3	1	3	2	2	0	2	1	9734.6831	-0.0080
3	1	3	3	2	0	2	2	9734.4170	-0.0026
3	1	3	4	2	0	2	3	9734.6831	-0.0049
3	2	2	2	2	1	1	1	15107.1305	0.0030
3	2	2	3	2	1	1	2	15106.9090	-0.0021
3	2	2	4	2	1	1	3	15107.0502	-0.0001
3	2	1	2	2	1	2	1	15270.1172	-0.0007
3	2	1	3	2	1	2	2	15271.0340	-0.0018
3	2	1	4	2	1	2	3	15270.4455	0.0022
4	0	4	3	3	1	3	2	7164.2625	-0.0015
4	0	4	4	3	1	3	3	7164.6003	-0.0005
4	0	4	5	3	1	3	4	7164.3876	0.0022
4	1	4	3	3	0	3	2	12045.4488	0.0036

4	1	4	4	3	0	3	3	12045.1037	0.0006
4	1	4	5	3	0	3	4	12045.4060	-0.0040
4	2	3	3	3	1	2	2	17442.2657	0.0003
4	2	3	4	3	1	2	3	17441.9923	0.0007
4	2	3	5	3	1	2	4	17442.2061	-0.0011
4	2	2	3	3	1	3	2	17772.9596	0.0015
4	2	2	4	3	1	3	3	17773.7247	-0.0008
4	2	2	5	3	1	3	4	17773.1682	0.0007
4	3	1	3	4	2	2	3	13223.0214	0.0006
4	3	1	5	4	2	2	5	13223.1034	0.0003
4	3	1	4	4	2	2	4	13223.4259	0.0029
5	0	5	4	4	1	4	3	9671.7458	-0.0056
5	0	5	5	4	1	4	4	9672.0989	-0.0004
5	0	5	6	4	1	4	5	9671.8480	0.0033
5	1	5	4	4	0	4	3	14332.3234	0.0008
5	1	5	5	4	0	4	4	14331.9602	-0.0025
5	1	5	6	4	0	4	5	14332.2820	-0.0016
5	2	4	4	4	1	3	3	19750.4321	-0.0022
5	2	4	5	4	1	3	4	19750.1172	0.0018
5	2	4	6	4	1	3	5	19750.3815	0.0003
5	3	2	4	5	2	3	4	13210.6395	-0.0034
5	3	2	5	5	2	3	5	13210.8765	-0.0012
5	3	2	6	5	2	3	6	13210.6827	0.0001
6	0	6	5	5	1	5	4	12195.5920	-0.0060
6	0	6	6	5	1	5	5	12195.9399	0.0026
6	0	6	7	5	1	5	6	12195.6746	0.0032
6	1	6	5	5	0	5	4	16597.5565	0.0040
6	1	6	6	5	0	5	5	16597.1920	-0.0019
6	1	6	7	5	0	5	6	16597.5137	-0.0026
7	0	7	6	6	1	6	5	14732.1111	-0.0025
7	0	7	7	6	1	6	6	14732.4291	-0.0062
7	0	7	8	6	1	6	7	14732.1759	0.0037
7	1	7	6	6	0	6	5	18843.9416	0.0027
7	1	7	7	6	0	6	6	18843.5872	-0.0040
7	1	7	8	6	0	6	7	18843.9038	-0.0031
8	0	8	7	7	1	7	6	17277.2121	-0.0025
8	0	8	8	7	1	7	7	17277.5109	-0.0028
8	0	8	9	7	1	7	8	17277.2584	-0.0037

Table S6. Experimental transition frequencies of the observed parent species of conformer **II** of CO_2···IPA.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs} (MHz)	$\Delta\nu_{obs\text{-}calc}$ (MHz)
3	0	3	2	2	0	2	1	6358.8134	-0.0018
3	0	3	3	2	0	2	2	6358.9694	-0.0014
3	0	3	4	2	0	2	3	6359.0130	0.0010
3	1	3	2	2	1	2	1	6224.6841	0.0010
3	1	3	3	2	1	2	2	6224.4170	-0.0005
3	1	3	4	2	1	2	3	6224.7053	-0.0011
3	1	2	3	2	1	1	2	6504.9427	-0.0022
3	1	2	4	2	1	1	3	6505.2248	-0.0023
3	2	2	2	2	2	1	1	6366.6801	0.0021
3	2	2	3	2	2	1	2	6365.0850	0.0021
3	2	2	4	2	2	1	3	6366.1052	-0.0029
3	2	1	2	2	2	0	1	6373.6907	0.0013
3	2	1	3	2	2	0	2	6372.1004	0.0021
3	2	1	4	2	2	0	3	6373.1159	-0.0044
4	0	4	4	3	0	3	3	8470.2226	-0.0012
4	0	4	3	3	0	3	2	8470.1590	-0.0016
4	0	4	5	3	0	3	4	8470.2509	-0.0016
4	1	4	4	3	1	3	3	8297.1415	0.0010
4	1	4	3	3	1	3	2	8297.2299	0.0089
4	1	4	5	3	1	3	4	8297.2691	-0.0015
4	1	3	4	3	1	2	3	8671.2018	-0.0015
4	1	3	3	3	1	2	2	8671.2942	-0.0019
4	1	3	5	3	1	2	4	8671.3282	-0.0009
4	2	3	3	3	2	2	2	8486.5206	-0.0019
4	2	3	5	3	2	2	4	8486.4111	0.0005
4	2	3	4	3	2	2	3	8485.9755	0.0004
4	2	2	3	3	2	1	2	8504.0344	-0.0002
4	2	2	4	3	2	1	3	8503.4889	-0.0033
4	2	2	5	3	2	1	4	8503.9219	-0.0014
5	0	5	5	4	0	4	4	10574.3476	-0.0003
5	0	5	4	4	0	4	3	10574.3148	-0.0014
5	0	5	6	4	0	4	5	10574.3671	-0.0032
5	1	5	5	4	1	4	4	10367.8956	0.0000
5	1	5	4	4	1	4	3	10367.9295	0.0017
5	1	5	6	4	1	4	5	10367.9688	0.0010
5	1	4	5	4	1	3	4	10835.3933	-0.0006
5	1	4	4	4	1	3	3	10835.4360	0.0029
5	1	4	6	4	1	3	5	10835.4633	0.0000
5	2	3	4	4	2	2	3	10640.4036	-0.0038
5	2	3	5	4	2	2	4	10640.1655	0.0034
5	2	3	6	4	2	2	5	10640.3876	0.0027

5	3	3	4	4	3	2	3	10614.9807	0.0008
5	3	3	5	4	3	2	4	10614.3703	0.0008
5	3	3	6	4	3	2	5	10614.8636	0.0039
5	3	2	4	4	3	1	3	10615.4053	-0.0022
5	3	2	5	4	3	1	4	10614.7975	0.0002
5	3	2	6	4	3	1	5	10615.2890	0.0017
6	0	6	6	5	0	5	5	12669.7414	0.0026
6	0	6	7	5	0	5	6	12669.7552	-0.0027
6	1	6	6	5	1	5	5	12436.3314	-0.0059
6	1	6	5	5	1	5	4	12436.3558	0.0034
6	1	6	7	5	1	5	6	12436.3822	-0.0007
6	1	5	6	5	1	4	5	12996.9947	0.0012
6	1	5	5	5	1	4	4	12997.0066	-0.0067
6	1	5	7	5	1	4	6	12997.0371	-0.0001
6	2	5	5	5	2	4	4	12722.8506	-0.0011
6	2	5	6	5	2	4	5	12722.7144	-0.0014
6	2	5	7	5	2	4	6	12722.8506	-0.0013
6	2	4	5	5	2	3	4	12783.6810	0.0010
6	2	4	6	5	2	3	5	12783.5456	-0.0059
6	2	4	7	5	2	3	6	12783.6810	0.0002
6	3	4	5	5	3	3	4	12739.4654	-0.0013
6	3	4	6	5	3	3	5	12739.1358	0.0013
6	3	4	7	5	3	3	6	12739.4230	0.0010
6	3	3	5	5	3	2	4	12740.6060	-0.0012
6	3	3	6	5	3	2	5	12740.2780	0.0027
6	3	3	7	5	3	2	6	12740.5644	0.0019
7	0	7	6	6	0	6	5	14755.0193	-0.0042
7	0	7	7	6	0	6	6	14755.0371	0.0051
7	0	7	8	6	0	6	7	14755.0421	-0.0070
7	1	7	6	6	1	6	5	14502.1295	-0.0004
7	1	7	7	6	1	6	6	14502.1154	-0.0066
7	1	7	8	6	1	6	7	14502.1492	-0.0043
7	1	6	7	6	1	5	6	15155.3785	-0.0011
7	1	6	8	6	1	5	7	15155.4077	-0.0021
7	2	6	6	6	2	5	5	14838.2714	0.0091
7	2	6	7	6	2	5	6	14838.1818	0.0010
7	2	6	8	6	2	5	7	14838.2714	0.0022
7	2	5	6	6	2	4	5	14934.7610	-0.0016
7	2	5	7	6	2	4	6	14934.6897	0.0003
7	2	5	8	6	2	4	7	14934.7735	0.0034
7	3	5	6	6	3	4	5	14864.7556	-0.0025
7	3	5	7	6	3	4	6	14864.5584	0.0005
7	3	5	8	6	3	4	7	14864.7487	0.0074
7	3	4	6	6	3	3	5	14867.3152	-0.0086

7	3	4	7	6	3	3	6	14867.1285	0.0043
7	3	4	8	6	3	3	7	14867.3152	0.0080
8	0	8	7	7	0	7	6	16829.2436	0.0053
8	0	8	8	7	0	7	7	16829.2436	0.0020
8	0	8	9	7	0	7	8	16829.2592	0.0017
8	1	8	7	7	1	7	6	16564.9599	0.0073
8	1	8	8	7	1	7	7	16564.9491	0.0012
8	1	8	9	7	1	7	8	16564.9683	-0.0028
8	1	7	7	7	1	6	6	17309.8545	-0.0048
8	1	7	8	7	1	6	7	17309.8545	0.0027
8	1	7	9	7	1	6	8	17309.8738	-0.0005
8	2	7	7	7	2	6	6	16951.3473	-0.0068
8	2	7	8	7	2	6	7	16951.3017	0.0004
8	2	7	9	7	2	6	8	16951.3658	0.0031
8	2	6	7	7	2	5	6	17094.2211	-0.0040
8	2	6	8	7	2	5	7	17094.1868	0.0054
8	2	6	9	7	2	5	8	17094.2394	0.0052
8	3	6	7	7	3	5	6	16990.7886	-0.0060
8	3	6	8	7	3	5	7	16990.6626	-0.0026
8	3	6	9	7	3	5	8	16990.7886	-0.0010
8	3	5	7	7	3	4	6	16995.9195	-0.0029
8	3	5	8	7	3	4	7	16995.7912	-0.0025
8	3	5	9	7	3	4	8	16995.9195	0.0021
2	2	1	1	1	1	0	0	15349.5083	-0.0017
2	2	1	2	1	1	0	1	15349.7011	0.0067
2	2	1	3	1	1	0	2	15349.2377	0.0045
2	2	0	2	1	1	1	1	15445.0716	-0.0024
2	2	0	3	1	1	1	2	15444.4423	0.0032
3	1	3	2	2	0	2	1	9803.2208	-0.0038
3	1	3	3	2	0	2	2	9803.6129	-0.0038
3	1	3	4	2	0	2	3	9803.4828	0.0001
3	2	2	2	2	1	1	1	17377.3694	0.0029
3	2	2	3	2	1	1	2	17378.0231	0.0019
3	2	2	4	2	1	1	3	17377.6029	0.0024
3	2	1	2	2	1	2	1	17666.4535	-0.0034
3	2	1	3	2	1	2	2	17667.4035	-0.0013
3	2	1	4	2	1	2	3	17666.7981	0.0033
4	1	4	3	3	0	3	2	11741.6306	0.0003
4	1	4	4	3	0	3	3	11741.7834	-0.0030
4	1	4	5	3	0	3	4	11741.7433	0.0021
4	2	3	3	3	1	2	2	19358.6495	-0.0005
4	2	3	4	3	1	2	3	19359.0551	0.0037
4	2	3	5	3	1	2	4	19358.7888	0.0047
4	2	2	3	3	1	3	2	19945.7985	-0.0099

4	2	2	4	3	1	3	3	19946.4778	-0.0017
4	3	1	3	4	2	2	3	18565.6218	-0.0018
4	3	1	5	4	2	2	5	18565.8325	0.0011
4	3	1	4	4	2	2	4	18566.6377	-0.0018
5	0	5	4	4	1	4	3	7302.8522	0.0058
5	0	5	6	4	1	4	5	7302.8886	0.0071
5	1	5	4	4	0	4	3	13639.3977	0.0001
5	1	5	5	4	0	4	4	13639.4571	-0.0010
5	1	5	6	4	0	4	5	13639.4571	0.0005
6	1	6	6	5	0	5	5	15501.4495	0.0020
6	1	6	7	5	0	5	6	15501.4659	-0.0033
7	0	7	7	6	1	6	6	11923.3298	0.0065
7	0	7	8	6	1	6	7	11923.3348	-0.0029
7	1	7	6	6	0	6	5	17333.8470	0.0052
7	1	7	7	6	0	6	6	17333.8262	-0.0045
7	1	7	8	6	0	6	7	17333.8640	-0.0009
8	0	8	8	7	1	7	7	14250.4408	-0.0021
8	0	8	9	7	1	7	8	14250.4408	-0.0009

Table S7. Experimental transition frequencies of the observed $^{14}N1$ isotopic species of isomer **I** of $CO_2\cdots$IPA.

J'	K_a'	K_c'	J''	K_a''	K_c''	ν_{obs} (MHz)	$\Delta\nu_{obs\text{-}calc}$ (MHz)
4	0	4	3	0	3	9632.8299	-0.0043
4	1	4	3	1	3	9526.7292	-0.0027
4	1	3	3	1	2	9753.3548	-0.0016
5	0	5	4	0	4	12033.8352	0.0014
5	1	5	4	1	4	11906.4172	0.0032
5	1	4	4	1	3	12189.5504	0.0023

Table S8. Experimental transition frequencies of the observed ^{13}C2 isotopic species of isomer **I** of $CO_2 \cdots$IPA.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs} (MHz)	$\Delta\nu_{obs-calc}$ (MHz)
4	1	4	4	3	1	3	3	9478.3893	0.0027
4	1	4	5	3	1	3	4	9478.4491	-0.0033
5	0	5	4	4	0	4	3	11966.0464	-0.0012
5	0	5	5	4	0	4	4	11966.0464	0.0041
5	0	5	6	4	0	4	5	11966.0671	-0.0015
5	1	5	4	4	1	4	3	11846.2447	-0.0086
5	1	5	5	4	1	4	4	11846.2447	-0.0022
5	1	5	6	4	1	4	5	11846.2926	0.0059
4	1	3	4	3	1	2	3	9689.4442	0.0037
4	1	3	5	3	1	2	4	9689.4860	-0.0036

Table S9. Experimental transition frequencies of the observed ^{13}C4(^{13}C5) isotopic species of isomer **I** of CO_2···IPA.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs} (MHz)	$\Delta\nu_{obs\text{-}calc}$ (MHz)
3	0	3	2	2	0	2	1	7169.5697	0.0079
3	0	3	3	2	0	2	2	7169.6122	-0.0046
3	0	3	4	2	0	2	3	7169.6372	-0.0061
4	0	4	3	3	0	3	2	9556.1484	0.0101
4	0	4	4	3	0	3	3	9556.1484	-0.0027
4	0	4	5	3	0	3	4	9556.1705	-0.0051
4	1	4	4	3	1	3	3	9464.7273	-0.0015
4	1	4	5	3	1	3	4	9464.7918	-0.0025
5	0	5	4	4	0	4	3	11939.8438	-0.0031
5	0	5	5	4	0	4	4	11939.8438	0.0008
5	0	5	6	4	0	4	5	11939.8641	-0.0039
5	1	5	4	4	1	4	3	11829.3839	-0.0057
5	1	5	5	4	1	4	4	11829.3839	0.0004
5	1	5	6	4	1	4	5	11829.4210	-0.0021
6	0	6	5	5	0	5	4	14320.0324	-0.0044
6	0	6	7	5	0	5	6	14320.0564	0.0061
6	1	6	5	5	1	5	4	14193.0358	0.0049
6	1	6	6	5	1	5	5	14193.0358	0.0087
6	1	6	7	5	1	5	6	14193.0572	0.0025
4	1	3	4	3	1	2	3	9657.9217	-0.0040
4	1	3	5	3	1	2	4	9657.9707	-0.0038
5	1	4	4	4	1	3	3	12070.8167	0.0017
5	1	4	5	4	1	3	4	12070.7837	0.0016
5	1	4	6	4	1	3	5	12070.8167	0.0064
5	2	4	5	4	2	3	4	11950.7697	0.0033
5	2	4	6	4	2	3	5	11950.8666	0.0011
5	2	4	4	4	2	3	3	11950.8666	-0.0092

Table S10. Experimental transition frequencies of the observed ^{13}C14 isotopic species of isomer **I** of CO_2···IPA.

J'	K_a'	K_c'	F'	J''	K_a''	K_c''	F''	ν_{obs} (MHz)	$\Delta\nu_{obs\text{-}calc}$ (MHz)
4	0	4	3	3	0	3	2	9560.9942	0.0062
4	0	4	4	3	0	3	3	9560.9942	-0.0055
4	0	4	5	3	0	3	4	9561.0210	-0.0041
4	1	4	4	3	1	3	3	9462.4334	0.0000
4	1	4	5	3	1	3	4	9462.4967	-0.0024
5	0	5	4	4	0	4	3	11945.1605	0.0006
5	0	5	5	4	0	4	4	11945.1605	0.0058
5	0	5	6	4	0	4	5	11945.1790	-0.0019
5	1	5	4	4	1	4	3	11826.3354	-0.0047
5	1	5	5	4	1	4	4	11826.3354	0.0017
5	1	5	6	4	1	4	5	11826.3777	0.0042
5	1	4	4	4	1	3	3	12087.6199	-0.0036
5	1	4	5	4	1	3	4	12087.5934	0.0032
5	1	4	6	4	1	3	5	12087.6199	0.0012

Table S11. Intensities (in arbitrary units) of the two isomers for several μ_a-type selected transitions.

Transitions	F' ←F"	Conformer	Frequencies	Intensities
3_{03}←2_{02}	4←3	I	7244.1548	0.057
		II	6359.0155	0.023
4_{04}←3_{03}	5←4	I	9654.9196	0.157
		II	8470.2508	0.052
4_{14}←3_{13}	5←4	I	9554.8774	0.040
		II	8297.2692	0.025
5_{05}←4_{04}	6←5	I	12062.3343	0.105
		II	10574.3360	0.058
7_{17}←6_{16}	8←7	I	16712.0049	0.008
		II	14502.1502	0.002
8_{08}←7_{07}	9←8	I	19257.1024	0.016
		II	16829.2515	0.004

Table S12. The percentage differences between the experimental and theoretical rotational constants of the isomers **I** and **II** of CO_2···IPA adduct at the different levels of theory. [a)]

		Isomer I				Isomer II			
Methods	Basis sets	A (MHz)	B (MHz)	C (MHz)	Ave[b] (%)	A (MHz)	B (MHz)	C (MHz)	Ave[b] (%)
Exp.		3854.6000	1234.5063	1181.3414	-	4778.4169	1107.7740	1014.2971	-
MP2	6-311++G(d,p)	3831(0.6%)	1260(-2.0%)	1197(-1.3%)	1.3	4724(1.1%)	1125(-1.5%)	1083(-6.8%)	3.2
	6-311++G(2d,p)	3850(0.1%)	1262(-2.2%)	1200(-1.6%)	1.3	4777(0.0%)	1133(-2.3%)	1061(-4.6%)	2.3
	6-311++G(2df,2pd)	3872(-0.4%)	1275(-3.3%)	1212(-2.6%)	2.1	4802(-0.5%)	1144(-3.3%)	1074(-5.9%)	3.2
	6-311++G(3df,3pd)	3860(-0.1%)	1285(-4.1%)	1220(-3.3%)	2.5	4786-(0.2%)	1148(-3.6%)	1091(-7.6%)	3.8
	def2-TZVP	3882(-0.7)	1268(-2.7%)	1207(-2.2%)	1.9	4788(-0.2%)	1132(-2.2%)	1054(-3.9%)	2.1
	jun-cc-PVTZ	3862(-0.2%)	1266(-2.6%)	1203(-1.9%)	1.5	4789(-0.2%)	1134(-2.4%)	1058(-4.3%)	2.3
	aug-cc-PVTZ	3865(-0.3%)	1292(-4.7%)	1227(-3.8%)	2.9	4800(-0.4%)	1152(-4.0%)	1070(-5.5%)	3.3
B3LYP-D3(BJ)	6-311++G(d,p)	3873(-0.5%)	1291(-4.6%)	1232(-4.3%)	3.1	4780(0.0%)	1142(-3.1%)	1067(-5.2%)	2.8
	6-311++G(2d,p)	3872(-0.5%)	1277(-3.5%)	1219(-3.2%)	2.4	4789(-0.2%)	1134(-2.4%)	1057(-4.2%)	2.3
	6-311++G(2df,2pd)	3878(-0.6%)	1271(-3.0%)	1213(-2.7%)	2.1	4793(-0.3%)	1133(-2.3%)	1057(-4.2%)	2.3
	6-311++G(3df,3pd)	3870(-0.4%)	1274(-3.2%)	1215(-2.9%)	2.2	4793(-0.3%)	1131(-2.1%)	1055(-4.0%)	2.1
	def2-TZVP	3879(-0.6%)	1275(-3.3%)	1217(-3.0%)	2.3	4806(-0.6%)	1132(-2.2%)	1035(-2.1%)	1.6
	jun-cc-PVTZ	3873(-0.5%)	1267(-2.7%)	1209(-2.3%)	1.8	4788(-0.2%)	1127(-1.7%)	1050(-3.6%)	1.8
	aug-cc-PVTZ	3875(-0.5%)	1270(-2.9%)	1212(-2.6%)	2.0	4792(-0.3%)	1130(-2.0%)	1047(-3.2%)	1.8
B2PLYP-D3(BJ)	6-311++G(d,p)	3856(0.0%)	1275(-3.3%)	1214(-2.8%)	2.0	4772(0.1%)	1129(-1.9%)	1056(-4.1%)	2.0
	6-311++G(2d,p)	3862(-0.2%)	1267(-2.7%)	1207(-2.2%)	1.7	4784(-0.1%)	1128(-1.8%)	1049(-3.4%)	1.8
	6-311++G(2df,2pd)	3872(-0.5%)	1265(-2.5%)	1205(-2.0%)	1.7	4795(-0.3%)	1130(-2.0%)	1051(-3.6%)	2.0
	6-311++G(3df,3pd)	3862(-0.2%)	1272(-3.1%)	1211(-2.5%)	1.9	4793(-0.3%)	1130(-2.0%)	1052(-3.7%)	2.0

	def2-TZVP	3873(-0.5%)	1266(-2.6%)	1206(-2.1%)	1.7	4803(-0.5%)	1126(-1.6%)	1024(-1.0%)	1.0
	jun-cc-PVTZ	3865(-0.3%)	1259(-2.0%)	1199(-1.5%)	1.2	4788(-0.2%)	1123(-1.3%)	1041(-2.6%)	1.4
	aug-cc-PVTZ	3866(-0.3%)	1269(-2.8%)	1208(-2.3%)	1.8	4798(-0.4%)	1130(-2.0%)	1036(-2.1%)	1.5
	6-311++G(d,p)	3880(-0.7%)	1289(-4.4%)	1229(-4.0%)	3.0	4809(-0.6%)	1138(-2.8%)	1060(-4.5%)	2.6
	6-311++G(2d,p)	3879(-0.6%)	1275(-3.3%)	1215(-2.8%)	2.2	4813(-0.7%)	1129(-1.9%)	1052(-3.7%)	2.1
	6-311++G(2df,2pd)	3890(-0.9%)	1265(-2.5%)	1207(-2.2%)	1.9	4815(-0.8%)	1128(-1.9%)	1052(-3.8%)	2.1
ωB97XD	6-311++G(3df,3pd)	3878(-0.6%)	1270(-2.9%)	1210(-2.5%)	2.0	4810(-0.7%)	1118(-0.9%)	1044(-2.9%)	1.5
	def2-TZVP	3888(-0.9%)	1256(-1.8%)	1199(-1.5%)	1.4	4813(-0.7%)	1114(-0.6%)	1038(-2.3%)	1.2
	jun-cc-PVTZ	3881(-0.7%)	1249(-1.2%)	1191(-0.8%)	0.9	4804(-0.5%)	1113(-0.5%)	1040(-2.5%)	1.2
	aug-cc-PVTZ	3885(-0.8%)	1252(-1.4%)	1194(-1.1%)	1.1	4806(-0.6%)	1115(-0.6%)	1041(-2.6%)	1.3
CCSD	6-311++G(d,p)	3836(0.5%)	1236(-0.1%)	1178(0.3%)	0.3	4750(0.6%)	1102(0.5%)	1043(-2.9%)	1.3
	6-311++G(2d,p)	3853(0.1%)	1231(0.3%)	1173(0.7%)	0.3	4781(-0.1%)	1104(0.3%)	1028(-1.4%)	0.6

a) The values in parentheses are percentage differences defined as: 100% × (experimental-theoretical)/experimental.

b) Average absolute percentage error for each level.

Table S13. Experimental (r_s and r_0) and theoretical (r_e) coordinates of the four C and one N atoms for the isomer **I** of CO_2···IPA adduct.

Atom		a (Å)	b (Å)	c (Å)
N1	r_s	±0.534(3) [a]	±1.164(11)	0.000 [b]
	r_0	-0.558(7)	1.166(8)	0.000
	r_e	-0.546	1.158	0.000
C2	r_s	±1.819(1)	±0.412(34)	0.000 [b]
	r_0	-1.822(6)	0.424(10)	0.000
	r_e	-1.804	0.407	0.000
C4	r_s	±1.866(2)	±0.434(8)	±1.256(3)
	r_0	-1.872(5)	-0.455(3)	-1.271(1)
	r_e	-1.871	-0.446	-1.257
C5	r_s	±1.866(2)	±0.434(8)	±1.256(3)
	r_0	-1.872(5)	-0.455(3)	1.271(1)
	r_e	-1.871	-0.446	1.257
C14	r_s	±2.028(1)	±0.283(31)	0.000 [b]
	r_0	2.013(1)	-0.238(1)	0.000
	r_e	2.002	-0.237	0.000

a) Constain's errors expressed in parentheses in units of the last digit.

b) c-coordinates are fixed at zero by symmetry.

Table S14. Partial r_0 and calculated geometry at ωB97XD/jun-cc-pVTZ level of isomer **I**.

Bond lengths (Å)		Valence angles (°)		Dihedral angles (°)	
C2N1	1.465				
H3C2	1.099	H3C2N1	111.4		
C4C2	**1.546(8)** [a)]	C4C2H3	**109.1(9)**	C4C2H3N1	-119.6
C5C2	**1.546(8)**	C5C2H3	**109.1(9)**	C5C2H3N1	119.6
H6C4	1.090	H6C4C2	110.7	H6C4C2H3	-58.1
H7C4	1.092	H7C4C2	111.1	H7C4C2H3	61.6
H8C4	1.090	H8C4C2	110.2	H8C4C2H3	-178.4
H9C5	1.090	H9C5C2	110.7	H9C5C2H3	-58.1
H10C5	1.092	H10C5C2	111.1	H10C5C2H3	-61.6
H11C5	1.090	H11C5C2	110.2	H11C5C2H3	178.4
H12N1	1.012	H12N1C2	110.8	H12N1C2H3	59.1
H13N1	1.012	H13N1C2	110.8	H13N1C2H3	-59.1
C14N1	**2.929(13)**	C14N1C2	**121.0(9)**	C14N1C2H3	180.0
O15C14	1.157	O15C14N1	**92.8(6)**	O15C14N1C2	0.0
O16C14	1.157	O16C14O15	175.9	O16C14O15C2	180.0

a) Error in parentheses in units of the last digit. The parameters in bold have been adjusted to reproduce the experimental values of rotational constants. Their theoretical values are 1.521 Å, 108.0°, 1.521 Å, 108.0°, 2.905 Å, 120.5° and 94.1°, respectively.

Table S15. Partial r_0 and calculated geometry at ωB97XD/jun-cc-pVTZ level of isomer **II**.

Bond lengths (Å)		Valence angles (°)		Dihedral angles (°)	
C2N1	1.464				
H3C2	1.093	H3C2N1	106.3		
C4C2	1.528	C4C2H3	108.5	C4C2H3N1	-122.5
C5C2	1.521	C5C2H3	108.1	C5C2H3N1	116.7
H6C4	1.091	H6C4C2	111.3	H6C4C2N1	-177.1
H7C4	1.091	H7C4C2	111.0	H7C4C2N1	-56.8
H8C4	1.093	H8C4C2	110.4	H8C4C2N1	63.0
H9C5	1.090	H9C5C2	110.9	H9C5C2C4	-56.7
H10C5	1.089	H10C5C2	110.8	H10C5C2C4	-177.3
H11C5	1.093	H11C5C2	110.5	H11C5C2C4	62.7
H12N1	1.013	H12N1C2	110.3	H12N1C2C4	-65.5
H13N1	1.012	H13N1C2	110.6	H13N1C2C4	52.2
C14N1	**2.916(4)** [a)]	C14N1C2	111.3	C14N1C2C4	169.1
O15C14	1.158	O15C14N1	90.6	O15C14N1C2	**-14.5(12)** [a)]
O16C14	1.157	O16C14O15	176.5	O16C14O15N1	178.5

a) Error in parentheses in units of the last digit. The parameters in bold have been adjusted to reproduce the experimental values of rotational constants. Their theoretical values are 2.877 Å and -22.3 °, respectively.

Table S16. Stabilization energy contributions (≥ 0.21 kJ/mol) for the isomer **I** of the CO_2···IPA adduct.

Donor NBO	Acceptor NBO	E(2) [kJ/mol]
From IPA to CO_2		
BD (1) C2 – N4	RY*(1) C5	0.21
LP (1) N4	RY* (4) C5	0.29
LP (1) N4	RY* (3) O7	0.25
LP (1) N4	BD*(1) C5 – O6	0.33
LP (1) N4	**BD*(3) C5 – O6**	**6.99**
From CO_2 to IPA		
BD (1) C5 – O6	RY*(3) N4	0.33
BD (3) C5 – O6	BD*(1) C2 – N4	0.59
LP (1) O7	RY*(3) H10	0.25
LP (1) O7	RY*(3) H13	0.25
LP (2) O7	**BD*(1) C1 – H10**	**0.46**
LP (2) O7	**BD*(1) C3 – H13**	**0.46**

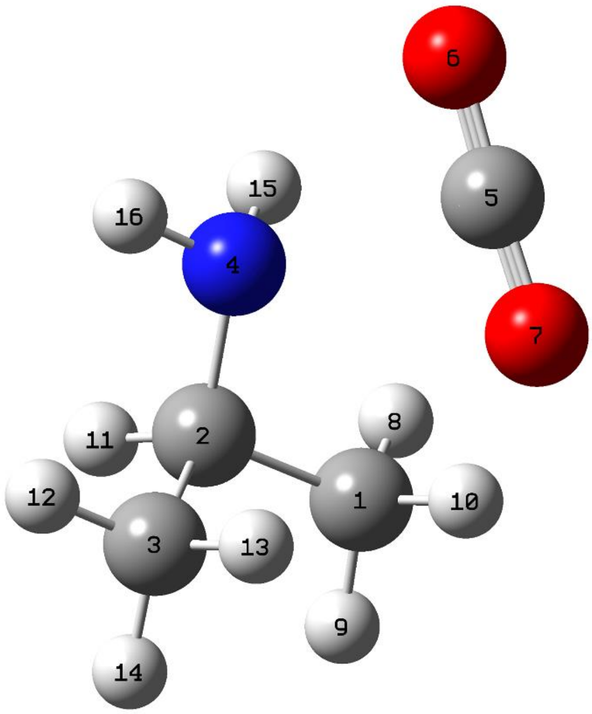

Table S17. Stabilization energy contributions (≥ 0.21 kJ/mol) for the isomer **II** of the CO_2···IPA adduct.

Donor NBO	Acceptor NBO	E(2) [kJ/mol]
From IPA to CO_2		
BD (1) C2 – N4	RY*(1) C5	0.25
LP (1) N4	RY* (4) C5	0.29
LP (1) N4	RY* (5) C5	0.29
LP (1) N4	RY* (3) O6	0.25
LP (1) N4	RY* (3) O7	0.21
LP (1) N4	BD*(1) C5 – O7	0.38
LP (1) N4	**BD*(3) C5 – O7**	**8.28**
From CO_2 to IPA		
BD (3) C5 – O7	RY*(1) N4	0.25
BD (3) C5 – O7	BD*(1) C2 – N4	0.29
LP (2) O6	BD*(1) C1 – C2	0.38
LP (3) O6	**BD*(1) C3 – H12**	**0.21**

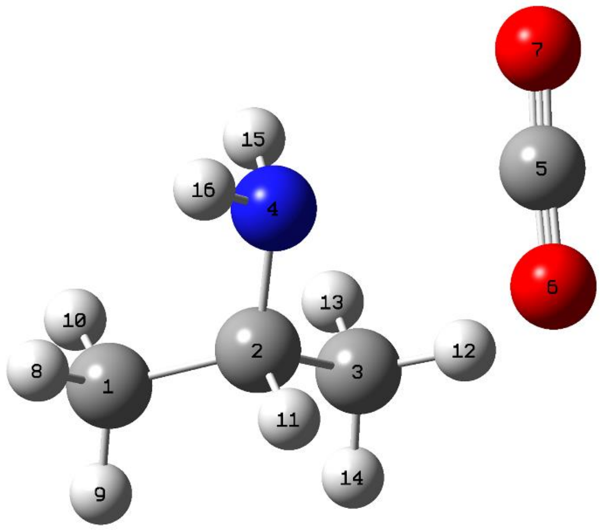

Table S18. NPA charges for the isomers **I** and **II** of CO_2···IPA adduct and CO_2 and IPA isolated molecules. Bold values highlight the values of the sulfur and fluorine atoms involved in the charge transfer.

	Isomer **I**	Isomer **II**	*Trans*	*Gauche*	CO_2
C	-0.585	-0.591	-0.581	-0.592	
C	-0.031	-0.038	-0.032	-0.034	
C	-0.585	-0.582	-0.581	-0.581	
N	**-0.851**	**-0.842**	**-0.840**	**-0.831**	
H	0.194	0.196	0.195	0.196	
H	0.202	0.201	0.200	0.199	
H	0.208	0.192	0.203	0.191	
H	0.147	0.176	0.144	0.169	
H	0.194	0.209	0.195	0.210	
H	0.208	0.189	0.203	0.189	
H	0.202	0.203	0.200	0.199	
H	0.352	0.345	0.348	0.339	
H	0.353	0.350	0.348	0.346	
C	**1.009**	**1.008**			**0.987**
O	-0.507	-0.512			-0.493
O	-0.509	-0.505			-0.493

Table S19. Results of the SAPT analysis for the isomers **I** and **II** of CO_2···IPA, and compared with the complexes of CO_2 with eight nitrogen-containing compounds [a].

Complexes	NCIs [b]	Distances	E_{elec}	E_{ind}	E_{disp}	E_{ex}	E_t
CO_2···IPA-**I**	C···N	2.929 [c]	-30.6(61%) [d]	-4.4(9%)	-15.0(30%)	29.1	-20.9
CO_2···IPA-**II**	C···N	2.916 [c]	-30.5(61%)	-4.7(9%)	-14.5(29%)	28.9	-20.8
CO_2···HCN	C···N	2.998 [c]	-10.7(58%)	-1.6(9%)	-6.3(34%)	7.9	-10.7
CO_2···NH_3	C···N	2.9875 [c]	-24.4(67%)	-3.5(10%)	-8.5(23%)	20.4	-16.0
CO_2···MA [e]	C···N	2.881 [f]	-29.2(64%)	-4.4(10%)	-11.8(26%)	26.3	-19.1
CO_2···EA [e]	C···N	2.881 [f]	-29.9(62%)	-4.6(9%)	-14.1(29%)	28.3	-20.3
CO_2···NPA [e]	C···N	2.878 [f]	-30.0(61%)	-4.7(9%)	-14.8(30%)	28.8	-20.7
CO_2···Py	C···N	2.7977 [c]	-31.3(62%)	-5.0(10%)	-14.5(29%)	26.5	-24.3
CO_2···FM-**I**	C···O	2.836 [c]	-32.7(61%)	-7.1(13%)	-13.8(26%)	27.4	-26.2
CO_2···FM-**II**	C···O	2.789 [c]	-26.6(62%)	-4.9(11%)	-11.6(27%)	21.0	-22.1

a) All the values are given in kJ mol^{-1}. b) NCIs represent the type of non-covalent interactions occurring in the complex. c) the values (in unit of Å) derive from the corresponding r_0 structures. d) The values in parenthesis are the contribution of each component with respect to the total attractive interaction (E_{elec} + E_{ind} + E_{disp}). e) only the most stable conformer is considered for these two conformers. f) Calculated at the ωB97XD/aug-cc-pVTZ level.