డాక్టర్ మొహమ్మద్ నయీమ్
భౌతిక శాస్త్ర అధ్యాపకులు
కె ఆర్ కె ప్రభుత్వ డిగ్రీ కళాశాల
అద్దంకి
ప్రకాశం జిల్లా
ఫోన్: 9866374987

అంతర్జాతీయ జర్నల్‌లో జిల్లా లెక్చరర్ల పరిశోధనా పత్రం

కరోనా వ్యాధి చికిత్సకు మందులను ఎంచుకునే సిద్ధాంత పత్రం ఆవిష్కరణ

అద్దంకి: అద్దంకి పట్టణంలోని కట్టారామకోటేశ్వర రావు డిగ్రీ అండ్ పీజీ కళాశాల లెక్చరర్ డాక్టర్ మహమ్మద్ నయీమ్, సర్వశిక్షా అభియాన్ ప్రకాశం జిల్లా ప్రాజెక్ట్ అధికారి (కందుకూరు ప్రభుత్వ కళాశాల రసాయన శాస్త్ర లెక్చరర్) డాక్టర్ శ్రీనివాసరెడ్డి సంయుక్తంగా కోవిడ్ వైరస్‌పై రెమ్ డెసివిర్ మందుతో చికిత్స చేసే విధానాన్ని గురించిన పరిశోధనాత్మక వ్యాసాన్ని రాశారు. ఈ వ్యాసం అంతర్జాతీయ ఎల్సెవిర్ జర్నల్, యూరోపియన్ జర్నల్ ఆఫ్ ఫార్మకాలజీలో ప్రచురితమైన సందర్భంగా విద్యాశాఖ మంత్రి ఆదిమూలపు సురేష్ ఆచార్యులను ఒంగోలులో నిర్వహించిన ఓ కార్యక్రమంలో గురువారం అభినందించారు. ఈ సందర్భంగా డాక్టరు నయీమ్ మాట్లాడుతూ ప్రపంచ వ్యాప్తంగా కరోనా వైరస్ వ్యాపించి లక్షల సంఖ్యలో మరణానికి కారణమైన నేపథ్యంలో వైరస్ కట్టడికి సరిపోయే మందులను ఎంచుకునే విధానాన్ని గురించిన పరిశోధన పత్రాన్ని భౌతిక రసాయన శాస్త్రాలను మేళవించి సిద్ధాంతీకరించినట్లు చెప్పారు. తాము పరిశోధించి తయారు చేసిన సిద్ధాంతం డబ్ల్యూహెచ్‌వో చికిత్సా విధివిధానాలకు సమానమైన ఫలితాలను ఇవ్వడం గమనార్హమని చెప్పారు. ఇదే సిద్ధాంతాన్ని మరి కొన్ని మందులపై ఉపయోగించగా వచ్చిన ఫలితాల పరిశోధనా పత్రాలు అంతర్జాతీయ ప్రొఫెసర్ల పరిశీలనలో ఉన్నాయని వివరించారు. ప్రపంచ వ్యాప్తంగా గుర్తింపు పొందిన ఈ పరిశోధనా పత్ర ఆవిష్కరణతో తాము ముందు ముందు మరిన్ని పరిశోధనలు చేయడానికి అవకాశం ఇచ్చిందన్నారు. పరిశోధనకు సహకరించిన డాక్టరు ఇర్షాద్ సోహైల్, డాక్టర్ ప్రియాంక సుదీర్‌కు అభినందనలు తెలియజేశారు.

లెక్చరర్‌లను అభినందిస్తున్న మంత్రి ఆదిమూలపు సురేష్

సాక్షి Fri, 16 October 2020
https://epaper.sakshi.com/c/55698046

ఆంధ్రప్రభ 8/8

పరిశోధనలతో రాష్ట్ర ఔన్నత్యం విశ్వవ్యాప్తం

- కరోనా వైరస్ చికిత్సకు రెమ్‌డెసివిర్ మందుపై పరిశోధనాత్మక వ్యాసం
- అధికారులను అభినందించిన మంత్రి

ఒంగోలు ఎడ్యుకేషన్, అక్టోబర్ 19(ప్రభన్యూస్): ప్రపంచాన్ని దేశాన్ని గడగడలాడిస్తున్న కరోనా మహమ్మారిపై రెమ్‌డెసివిర్ మందుతో చికిత్స గురించి పరిశోధనాత్మక వ్యాసాన్ని రాసినందుకు సమగ్ర శిక్ష అభియాన్ అదనపు ప్రాజెక్టు కో ఆర్డినేటర్, కందుకూరు ప్రభుత్వ డిగ్రీ కళాశాల రసాయన అధ్యాపకులు డాక్టర్ ఎం శ్రీనివాసరెడ్డి, అద్దంకి కెఆర్‌కె ప్రభుత్వ డిగ్రీ కళాశాల భౌతికశాస్త్ర అధ్యాపకులు మహమ్మద్ నయీమ్‌లను రాష్ట్ర విద్యాశాఖామంత్రి ఆదిమూలపు సురేష్ అభినందించారు. ఈ ప్రతిష్టాత్మక వ్యాసం యల్సేవిర్ జర్నల్ యురోపియన్ జర్నల్ ఆఫ్ ఫార్మకాలజీలో ప్రచురితమైనసందర్భంగా వారిద్దరిని అభినందించారు. అంతర్జాతీయ పరిశోధనాత్మక పత్రికలు, యల్సవిర్, అమెరికన్ కెమికల్ సొసైటీ, ట్యాలర్ అండ్ ఫ్రాన్సిస్ జర్నల్‌లలో 35 పత్రికలపైగా ఈ వ్యాసాన్ని ప్రచురించడం చేశారన్నారు. యూనివర్సిటీలు, రీసెర్చ్ సెంటర్లకు కూడా సాధ్యం కాని ఈ పరిశోధన ఫలాలతో ఆంధ్రప్రదేశ్ రాష్ట్ర ఔన్నత్యం విశ్వవ్యాప్తమైందని చెప్పారు. ప్రపంచ వ్యాప్తంగా కరోనా విజృంభించి అన్ని దేశాలను పట్టి పీడిస్తూ లక్షాలాది మరణాలకు దారి తీయడమే కాకుండా దీని నుంచి కోలుకున్న వారి ఆరోగ్యంపై చాలా వరకు దుష్ప్రభావాన్నిచూపిస్తూ ఆర్థికంగా, మానసికంగా దెబ్బతీస్తున్న ఈ మహమ్మారి చికిత్సకు సరిపోయే మందులను ఎలా ఎంచుకోవాలో ఈ పత్రంలో సిద్ధాంతీకరించడం జరిగిందన్నారు. అత్యాధునిక కాంపిటేషన్ పద్ధతియను భౌతిక రసాయన శాస్త్ర సిద్ధాంతాలకు మేళవించి జిల్లా వాసులు కనుగొన్న సిద్ధాంతం ప్రపంచ దేశాలతో పాటు డబ్ల్యూహెచ్‌ఓ చికిత్స విధి విధానాలకు తుల్యమైన ఫలితాలతో సరిపోవడం విశేషమని డాక్టర్ నయీమ్ పేర్కొన్నారు. ఇదే సిద్ధాంతాన్ని ఇతర మందుల్ని ఉపయోగించి చేసిన తమ పరిశోధన పత్రాలు అంతర్జాతీయ ప్రొఫెసర్ల పరిశీలనలో ఉన్నాయన్నారు. దేశ వ్యాప్తంగా అత్యధిక కోవిడ్ -19 పరీక్షలు చేస్తూ డబ్ల్యూహెచ్‌ఓ నిబంధనలకు అనుగుణంగా కోవిడ్ చికిత్సకు సంబంధించిన వివిధ విధానాలను పాటిస్తున్న రాష్ట్రప్రభుత్వానకు ప్రత్యేక అభినందనలు తెలిపారు. ఈ పరిశోధనాత్మక పత్రం ప్రకాశం జిల్లాలోని కందుకూరు, అద్దంకి, కళాశాలలకు ప్రభుత్వానికి గర్వకారణమన్నారు. కొత్త సిద్ధాంతాల ఆవిష్కరణ చేసే నిత్య పరిశోధకులు డాక్టర్ నయీమ్, డాక్టర్ ఎం శ్రీనివాసరెడ్డి విశేష పరిశోధనలకు రాష్ట్రప్రభుత్వం సముచిత స్థానం అందిస్తుందని విద్యాశాఖామంత్రి ఆదిమూలపు సురేష్ ఆశాభావం వ్యక్తం చేశారు. కరోనా నియంత్రణకు వాడుతున్న మందులలో రెమ్‌డెసివిర్ అత్యంత ప్రభావశీలంగా ఉందని అమెరికన్ వైద్యుల పరిశోధనలో కూడా వెల్లడైందన్నారు.

ఏపీసీని అభినందిస్తున్న మంత్రి ఆదిమూలపు సురేష్

ప్రమోషన్ పోస్టులను ఖాళీలుగా చూపాలి

1200 లీటర్ల బెల్లంఊట ధ్వంసం

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

ఈనాడు
epaper.eenadu.net

అభినందనీయం.. పరిశోధనా వ్యాసం

ఒంగోలు నగరం, న్యూస్‌టుడే: జిల్లాకు చెందిన ఇద్దరు ప్రభుత్వ డిగ్రీ కళాశాల అధ్యాపకులు కొవిడ్ చికిత్సలో వినియోగిస్తున్న రెమీ డెసివర్ మందు వినియోగంపై రాసిన పరిశోధనాత్మక వ్యాసానికి గుర్తింపు లభించింది. సమగ్రశిక్షా అభియాన్ ఏపీసీగా పనిచేస్తున్న కందుకూరు కళాశాల రసాయన శాస్త్ర అధ్యాపకుడు శ్రీనివాసరెడ్డి, అద్దంకి కళాశాల భౌతికశాస్త్ర అధ్యాపకుడు మహ్మద్ నయీమ్ సంయుక్తంగా ఈ వ్యాసం రాశారు. అంతర్జాతీయ ఎల్సేవిర్ జర్నల్ యూరోపియన్ జర్నల్ ఆఫ్ ఫార్మకాలజీలో ప్రచురితమైంది. ఒంగోలులో విద్యాశాఖ మంత్రి ఆది మూలపు సురేష్‌కు ఆ వ్యాసాన్ని గురువారం అందజేశారు. ఇద్దరు అధ్యాపకులను మంత్రి అభినందించారు.

Date : 16/10/2020 EditionName : ANDHRA PRADESH(PRAKASAM)
PageNo : 05

16/05/2021-

ప్రజాశక్తి
www.prajasakti.com

కెఆర్‌కె డిగ్రీ కళాశాల అధ్యాపకులు

మొహమ్మద్ నయీమ్‌కు అరుదైన గౌవరం

ప్రజాశక్తి- అద్దంకి

శంగరకొండ కెఆర్‌కె ప్రభుత్వ డిగ్రీ కళాశాల భౌతికశాస్త్ర అధ్యాపకులు డాక్టర్ మహమ్మద్ నయీమ్‌కు అరుదైన గౌవరం దక్కింది. 'కోవిడ్ వైరస్‌పై దాడికి ఔషధాలను ఎంచుకునే పద్ధతి' అనే అంశం గురించి ఆయన చేసిన పరిశోధనను అంతర్జాతీయ టేలర్ అండ్ ఫ్రాన్సిస్-ఇంగ్లాండ్ జర్నల్ దాదాపు 8 నెలలు పరిశీలన అనంతరం నయీమ్ పరిశోధనను ప్రపంచ వ్యాప్తంగా విడుదల చేసింది. ఈ సందర్భంగా నయీమ్ మాట్లాడుతూ అంపశయ్యపై కరోనా కరాళ నృత్యం చేస్తూ విశ్వ వ్యాప్తంగా కరోనా రెండవ దశ విజృంభించి ధనిక, పేద


మొహమ్మద్ నయీమ్

దేశాలను పట్టి పీడిస్తూ లక్షలాది మరణాలకు దారి తీరిసినట్లు తెలిపారు. కరోనా నుంచి కోలుకున్న ఆరోగ్యం పై చాలా కాలం వరకూ దుష్ప్రభావాన్ని చూపించి ఆర్థికంగా, మానసికంగా దెబ్బ తీస్తూ బతుకు ఛిద్రం చేస్తున్న కరోనా చికిత్సకు సరిపోయే ఔషధాలను ఎలా ఎంచుకోవాలనే అనే విషయాలను ఆ పత్రంలో తాను సిద్ధాంతీకరించి, రుజువు పరిచినట్లు తెలిపారు. అత్యాధునిక కంప్యూటేషన్ ప్రక్రియ, భౌతిక రసాయన సిద్ధాంతాలకు మేళవించి తాను కనుగొన్న విధానం ప్రపంచ దేశాలతో పాటు దమ్మాహెచ్ఓ చికిత్స మార్గదర్శకాలకు తుల్యమైన ఫలితాలతో సరిపోవడం విశేషం నయీమ్ పేర్కొన్నారు. సిద్ధాంతాన్ని పరిశీలించటానికి మరికొన్ని ఔషధాలపై ఉపయోగించి చేసిన తమ పరిశోధనలలో మొదటిది అత్యధిక డిమాండ్ ఉన్న రెమిడెసివర్ చికిత్స గురించిన పరిశోధన అంతర్జాతీయ ఎల్సేవిర్ జర్నల్- "యూరోపియన్ జర్నల్ ఆఫ్ ఫార్మకాలజీ' (యూరోప్)లో ప్రచురితమైనట్లు తెలిపారు. రెమిడెసివర్‌కు ప్రత్యామ్నాయంగా ఉపయోగ పడే 'డెక్సామిధజోన్' ఔషధం గురించి స్ప్రింగర్ జర్నల్- "రీసెర్చ్ ఆన్ బయో మెడికల్ ఇంజనీరింగ్" (బ్రెజిల్-యూస్ఏ)లో గత ఏడాదే ప్రచురితమైనట్లు తెలిపారు. ఈ సందర్భంగా ప్రభుదాస్, కమల బాబు, తిరుపతి స్వామి, రమేష్ తదితర ప్రముఖులు నయీమ్‌ను అభినందించారు.

Sun, 16 May 2021
epaper.prajasakti.com/c/60477714

V. Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

కేఆర్‌కే అధ్యాపకునికి అంతర్జాతీయ సైంటిస్ట్ ర్యాంక్

అద్దంకి: అంతర్జాతీయంగా ఏడీ సైంటిఫిక్ ర్యాంకింగ్స్ వారు శుక్రవారం విడుదల చేసిన సైంటిస్ట్ ర్యాంకింగ్స్‌లో పట్టణంలోని కట్టా రామకోటేశ్వరరావు ప్రభుత్వ డిగ్రీ అండ్ పీజీ కళాశాల భౌతిక శాస్త్ర అధ్యాపకుడు ఎస్‌కే అబ్దుల్ నయీమ్ మూడు స్థాయిల్లో వివిధ ర్యాంకులు పొందారు. ఈ ర్యాంకులను లింక్డ్ ఇన్, గుగూల్ స్కాలర్, స్టాన్‌ఫర్డ్ యూనివర్శిటీలు సంయుక్తంగా ప్రకటించినట్లు నయీమ్ శనివారం తెలిపారు. ఇందుకుగాను ఆయనకు ఏడీ సైంటిఫిక్ ర్యాంకింగ్స్ వారు ధ్రువపత్రాన్ని పంపారు. ఇందులో నయీమ్‌కు భౌతిక శాస్త్రంలో ఇండియా స్థాయిలో 6,256 ర్యాంకు, ఆసియాలో 25,904, వరల్డ్‌లో 1,03,108 వ ర్యాంకు, నాచురల్ సైన్స్‌లో ఇండియాలో 1,903, ఆసియాలో 7,498, వరల్డ్‌లో 27,528 ర్యాంకులు వచ్చాయి. అంత

నయీమ్‌ను అభినందిస్తున్న ప్రిన్సిపాల్, అధ్యాపకులు

ఐదు సంవత్సరాలుగా వివిధ పరిశోధనలు, కొత్త సిద్ధాంతాల ఆవిష్కరణలు, ఇతర శాస్త్రవేత్తలు తమ పరిశోధనలో సమర్థించిన అంశాల ప్రాతిపదికన ఈ ర్యాంకులు నిర్ణయిస్తారు. నయీమ్ భౌతికశాస్త్రం, నాచురల్ సైన్స్ రెండు సబ్జెక్టుల్లోనూ విశేష ప్రతిభ కనబరచి ర్యాంకులు పొందటం విశేషం. ఈయన నుంచి కోవిడ్‌పై చేసిన పరిశోధనలతో ప్రపంచ ఖ్యాతి పొందిన శాస్త్రవేత్తల ప్రశంసలు పొందారు. నలభైకి పైగా పరిశోధనా పత్రాలు ప్రపంచ ప్రఖ్యాత ఎల్స్‌వేర్, స్ప్రింగర్, టేలర్ అండ్ ఫ్రాన్సిస్, అమెరికన్ కెమికల్ సొసైటీల్లో ప్రచురితమయ్యాయి. స్వీడన్, అమెరికా, ఫ్రాన్స్, యూకేలకు చెందిన అంతర్జాతీయ పరిశోధన పత్రికలకు ఆయన పరిశీలకునిగా ఉన్నారు. అద్దంకి ప్రభుత్వ కళాశాలలో అంతర్జాతీయ సైన్స్ సెమినార్‌ను నిర్వహించి ఎంతో మంది విద్యార్థుల ఉన్నత చదువులకు మార్గదర్శకునిగా నిలిచారు. నయీమ్‌కు అంతర్జాతీయ సైంటిస్ట్ ర్యాంకు రావడంతో కళాశాల అధ్యాపకులు ఆయన్ను ఘనంగా శనివారం సన్మానించారు. ఈ సన్మాన కార్యక్రమంలో కేఆర్‌కే కళాశాల ప్రిన్సిపాల్ మోహన్‌రావు, డాక్టర్ భానూ అశోక్, రాజశేఖర్, డాక్టర్ అనిత, డాక్టర్ ప్రసాద్, ప్రభుదాస్

మీ ప్రాంతంలో
ో ఉన్నారు.
శ్రద్ధాంజలి,
నిర్వాణము,
వర్ధంతి
మొదలగు
రు సంప్రదించండి.
31
(అద్దంకి)
omail.com

సైన్స్ పరిశోధకుడు డాక్టర్ నయూంకు సత్కారం

అద్దంకి, న్యూస్‌టుడే: భౌతిక, రసాయన శాస్త్ర పరిశోధనల ద్వారా ప్రశంసలు అందుకున్న అధ్యాపకుడు డాక్టర్ మహమ్మద్ నయూం అని కేఆర్కే ప్రభుత్వ డిగ్రీ కళాశాల ప్రధానాచార్యుడు డాక్టర్ వి.మోహనరావు పేర్కొన్నారు. కళాశాలలో శనివారం నిర్వహించిన కార్యక్రమంలో ఆయనను సత్కరించారు. ఈ సందర్భంగా మాట్లాడుతూ గత రెండేళ్లుగా కొవిడ్‌పై ఆయన చేసిన పరిశోధనలు ప్రముఖ శాస్త్రవేత్తల ప్రశంసలు పొందాయన్నారు. నలభైకి పైగా పరిశోధన పత్రాలు ప్రముఖ జర్నల్‌లలో ప్రచురితమయ్యాయన్నారు. కళాశాలలో సైన్స్ కార్యశాల నిర్వహించి విద్యార్థులకు మార్గదర్శిగా నిలిచారన్నారు. కార్యక్రమంలో డాక్టర్ భాను, డాక్టర్ అశోక్, డాక్టర్ రాజశేఖర్, డాక్టర్ అనిత, డాక్టర్ ప్రసాద్, డాక్టర్ ప్రభుదాస్ తదితరులు పాల్గొన్నారు.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

EENADU-11/9/2017

ప్రత్యేక కథనాలు

తడబడి, జీవితంలో నిలబడి...

ఆత్మగౌరవానికి ప్రతీక ఒకరు

అడ్డంకులను అధిగమించి మరొకరు

సమాజ శ్రేయోభిలాషులీ విద్యాధికులు

విద్యార్థులకు బోధన చేస్తున్న అధ్యాపకుడు మహ్మద్ నయీం

అడ్డంకి న్యూస్‌టుడే: జీవితం అందరికీ వడ్డించిన విస్తరి కాదు. చేసే వృత్తులూ నల్లేరుపై నడకలు కాదు. సమాజం నిత్యం ఎన్నో సవాళ్లను

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

విసురుతూనే ఉంటుంది. వాటిని ఎంత దీటుగా ఎదుర్కొని నిలిచామనే మనోస్థైర్యం పైనే మన మనుగడ ఆధారపడి ఉంటుంది. ఇందుకు ఈ ఇద్దరి జీవితాలు ఓ నిదర్శనం. సాఫీగా సాగిపోతున్న ఉద్యోగం జీవితంలో అడ్డంకులు ఎదురై కలవరపాటుకు గురి చేశాయి. విపత్కర పరిస్థితుల్లోనూ ఆత్మగౌరవాన్ని వదిలేందుకు ఇష్టపడక చేస్తోన్న వృత్తిని వీడి తన మనసుకు నచ్చిన పేరే వృత్తిని ఎంచుకున్నారు ఒకరు. ఆడపిల్లకు చదువెందుకు అంటూ విధించిన అడ్డంకులను అధిగమించి పది మందికి చదువు చెప్పే వృత్తిలో స్థిరపడ్డారు మరొకరు. ఒకవైపు తమ వృత్తి ధర్మాన్ని నిర్వర్తిస్తూనే.. మరో వైపు రేపటి పౌరులకూ మార్గదర్శకులుగా నిలిచి వారిని తీర్చిదిద్దుతున్నారు. అలా తమకు చేతనైనంతలో సమాజ శ్రేయస్సుకు పాటుపడుతున్నారు. వారే అద్దంకిలోని కేఆర్‌కే ప్రభుత్వ డిగ్రీ కళాశాలలో అధ్యాపకులుగా పని చేస్తున్న నయీం, ఇందిర అనే అధ్యాపకులు.

ఎంపీడీవో ఉద్యోగం వదిలి...

మహ్మద్ నయీంది గుంటూరు జిల్లా చిలకలూరిపేట. అధ్యాపకునిగా పని చేయాలనేది ఇతని కాంక్ష. శ్రీవెంకటేశ్వర విశ్వవిద్యాలయంలో పట్టభద్రుడైన తర్వాత గ్రూప్-1 పరీక్ష రాశారు. తన ప్రతిభతో అందులో ఎంపీడీవోగా ఎంపికయ్యారు. తెలంగాణ రాష్ట్రంలోని రామగుండం ఎంపీడీవోగా విధుల్లో

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

చేరారు. జీవితం సాఫీగా సాగిపోతోందనుకుంటున్న తరుణంలో ఆటుపోట్లు ఎదురయ్యాయి. అక్కడ వృత్తిలో అబద్దాలు ఆడటం, మోసపు మాటలు చెప్పటాన్ని జీర్ణించుకోలేకపోయారు. ఈ క్రమంలో తీవ్ర మానసిక ఒత్తిడిని ఎదుర్కొన్నారు. తన మనసు చెప్పినట్టుగా విధి నిర్వహణ చేయలేకపోయారు. ఈ క్రమంలో పరిస్థితులతో రాజీ పడలేక తాను చేస్తోన్న గ్రూప్-1 ఉద్యోగానికి ఆరు నెలలకే రాజీనామా చేశారు. అనంతరం నంద్యాలలోని ఓ ప్రైవేటు ఇంజినీరింగ్ కళాశాలలో సహాయ ఆచార్యునిగా భౌతిక శాస్త్ర విభాగంలో ఆరు సంవత్సరాలు పనిచేశారు. 2004లో ఏపీపీఎస్సీ ద్వారా జూనియర్ అధ్యాపకునిగా ఎంపికయ్యారు. శ్రీకాకుళం జిల్లా సోంపేటలో పనిచేశారు. 2011లో తిరిగి ఏపీపీఎస్సీ ద్వారా డిగ్రీ లెక్చరర్ పరీక్ష రాసి ఎంపికయ్యారు. తొలుత కడపలో మూడు సంవత్సరాల పాటు పని చేశారు. 2014 నుంచి అద్దంకి కేఆర్‌కే ప్రభుత్వ డిగ్రీకళాశాలలో పని చేస్తున్నారు.

ప్రచురితమైన వ్యాసాలు ఎన్నెన్నో...

అధ్యాపక వృత్తి తనకు సంతృప్తినిచ్చిందంటారు నయీం. చదువులో వెనుకబడిన వారిపై ప్రత్యేక దృష్టిసారించి శ్రద్ధ కనబరుస్తారు. వారు కూడా చదువుల్లో ప్రతిభ చూపేలా తర్ఫీదునిస్తుంటారు. ఈయన ఎన్నో రచనలూ చేశారు. అవి స్ప్రింగర్, ఎల్స్‌వేర్ వంటి వాటిల్లో ప్రచురితమయ్యాయి.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

ఇప్పటి వరకు 30 వ్యాసాలు ప్రచురితమయ్యాయి. 2003లో ఆంధ్రా విశ్వవిశ్వవిద్యాలయం నుంచి అవార్డు కూడా అందుకున్నారు. భౌతికశాస్త్రం అంటే కష్టం అనే భయాన్ని విద్యార్థుల నుంచి పోగొట్టి సంతోషంగా చదివేలా చేయాలనేది తన తన ఆకాంక్ష అని ఆయన వివరించారు.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

16న భౌతిక శాస్త్ర సదస్సు

అద్దంకి : కట్టా రామకోటేశ్వరరావు డీగ్రీ అండ్ పీజీ కళాశాలలో ఈ నెల 16,17 తేదీల్లో భౌతిక శాస్త్రంపై సెమినార్ నిర్వహించనున్నట్లు ప్రోగ్రామ్ కోఆర్డినేటర్ మహ్మద్ నయీన్ శుక్ర వారం తెలిపారు. కళాశాలలో శుక్రవారం గోడ

గులు

త్రికను ప్రిన్సిపాల్ జీ. రాజేశ్వరి ఆవిష్కరిం య. భౌతిక శాస్త్రం- ప్రస్తుత పోకడలు అనే శంపై పోలెండ్ దేశ భౌతిక శాస్త్ర మైకేల్ స్మీ, ర్జునా యూనివర్సిటీ ప్రొఫెసర్లు డీ. రావు, బి .వీరయ్య హాజరవుతున్నట్లు రు. అధ్యాపకులు ఇందిరా, సంపూర్ణ ల్గొన్నారు.

ప్రభుత్వం వైద్యశిబిరా ుకోవాలని ానూతలలో బీఎం ఆధ్వ వృద్ధి కార్య క్రమంలో భాగంగా నల్ప ంచిన వైద్య

పరిశోధన ఫలాలు పేదలకు అందాలి

అద్దంకి రూరల్: మేధావుల పరిశోధనా ఫలితాలు పేద ప్రజలు అందడమే ముఖ్య మని నాగార్జున యూనివర్శిటీ ప్రొఫెసర్ వీరయ్య అన్నారు. శింగరకొండ సమీపంలోని కె.ఆర్. కె. డిగ్రీ అండ్ పీజీ కళాశాలలో అధ్యా పకుడు నయూమ్ ఆధ్వర్యంలో నిర్వహించిన 'భౌతికశాస్త్రలో ఇటీవల వచ్చిన మార్పులు' అనే అంశంపై బుధవారం నిర్వహించిన సమావేశంలో మాట్లాడారు. ఐక్యరాజ్యసమితి ఈ ఏడాదిని కాంతి సంవత్సరంగా ప్రక టించాలన్నారు. భూభాగంపై ఎన్నో దేశాలు కాంతి లేకుండా చీకటిలోనే జీవిస్తున్నాయని చెప్పారు. గ్లాస్ సైన్సు, లేజర్స్,

మాట్లాడుతున్న వీరయ్య

యూమినిసైన్స్, అల్ట్రా సానిక్స్, ఇంటర్నెట్ అనువర్తనాల పరిశోధనల గురించి వివ రించారు. ఆర్.ఆర్. సెక్రి మాట్లాడుతూ ఇంటర్నెట్, ధర్మడైనమిక్స్ ప్రస్తుత పరివర్తన అనువర్తనల గురించి వివరించారు. విజయ వాడ ఇంజినీరింగ్ కాలేజీ ప్రొఫెసర్ గాంధీ, సహాయబాస్కర్‌లు బయోగ్లాసెస్ పరిశోధనల గురించి తెలిపారు. నెల్లూరు, కడప, కర్నూలు, చిత్తూరు జిల్లాల నుంచి దాదాపు 120 మంది వక్తలు పరిశోధనా ఫలితాల గురించి వివ రించారు. కళాశాల ప్రిన్సిపల్ శ్రీలక్ష్మి, పి. ఇందిరా, డీ. సంపూర్ణరావు పాల్గొన్నారు.

V. Lakshmi

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

భౌతిక శాస్త్రానిదే ప్రథమ స్థానం

ంకి రూరల్: ప్రపంచీకరణలో భౌతికశాస్త్రం ప్రథమ నంలో ఉందని పోలెండ్ దేశ భౌతిక శాస్త్ర ప్రొఫెసర్ మైఖేల్ యాకీ అన్నారు. యూ.జి.సి. సహకారంతో కె.ఆర్.కె మత్వ డిగ్రీ కళాశాలలో గురువారం 'అనువర్తిత భౌతికశా - సరికొత్త పోకడలు' అనేఅంశంపై రెండో రోజు జాతీయ స్సు నిర్వహించారు. కళాశాల ప్రిన్సిపాల్ రాజేశ్వరీ అధ్య వహించిన కార్యక్రమంలో మైఖేల్‌సీయాకీ మాట్లాడుతూ ువర్తిత భౌతికశాస్త్రంలో నేడు వస్తున్న మార్పులను ఎప్పటి ుడు తెలుసుకుని వాటికి అనుగుణంగా పరిశోధనలు ూలని సూచించారు. ప్రోగ్రామ్ కన్వీనర్ భౌతికశాస్త్ర అధ్యా లు మొహమ్మద్‌నయీమ్ మాట్లాడుతూ భౌతికశాస్త్ర అభి ద్ధి అనువర్తనాలు మత తత్వం, మూఢనమ్మకాలు అధిగ ంచిన రోజున దేశం ప్రగతి పథంలో పయనిస్తుందని ్పిరు. భారతీయార్ యూనివర్శిటీ ప్రొఫెసర్ జాన్‌పాల్, మసింహపురి యూనివర్శిటీ ప్రొఫెసర్ సురేష్, తెలంగా కు చెందిన సి.టి. కాలేజీ ప్రొఫెసర్ శ్రీనివాసరావు, కడప

మాట్లాడుతున్న పోలెండ్ శాస్త్ర మైఖేల్ సీయాకీ

జ్ఞాపికలు అందజేస్తున్న అధ్యాపకురాలు ఇందిర

గవర్నమెంట్ కాలేజీ ప్రొఫెసర్ జీ. శివరామయ్య తమ పరిశోధ నల ఫలితాలను వివరించారు. సదస్సులో 22 పరిశోధనా పత్రాలను ప్రదర్శించారు. మూఢనమ్మకాలపై బి.వి రామన్ నిర్వహించిన మేజిక్ షో అలరించింది. సదస్సులో పాల్గొన్నవా రికి ప్రశంసా పత్రాలను అందించారు. కళాశాల భౌతికశాస్త్ర అధ్యాపకులు పి.ఇందిరా, డి. సంపూర్ణరావు అధ్యాపక, అధ్యా పకేతర సిబ్బంది పాల్గొన్నారు.

ఆంధ్రజ్యోతి

రిశోధనలు సమాజానికి ఉపయోగపడాలి

పోలాండ్ డ్లూగోజ్ యూనివర్సిటీ భౌతికశాస్త్రం ప్రొఫెసర్ మైఖేల్ పియాసెఖి

ష్ణంకి టౌన్ : పరిశోధనలు సమాజం గ్రామీణ ప్రాంతాల ప్రజలకు కూడా ఉ గపడేల ఉండాలని, ఆ దిశగా పరిశోధ జరగాలని పోలాండ్ డ్లూగోజ్ యూనివ భౌతికశాస్త్రం ప్రొఫెసర్ మైఖేల్ పియా ఆచార్య నాగార్జున యూనివర్శిటీ ప్రొఫె ఎన్.వీరయ్య పేర్కొన్నారు. బుధవారం రకొండ వద్ద గల కేఆర్‌కే ప్రభుత్వ డిగ్రీ ాలలో యూజీసీ సహకారంతో కళా ఫిజిక్స్ డిపార్టుమెంట్ ఆధ్వర్యంలో భౌతి స్త్రంలో ఇటీవల వస్తున్న మార్పులపై జా ీయ సదస్సు జరిగింది. ఈ సందర్భంగా వా మాట్లాడుతూ 2015 సంవత్సరాన్ని యూ ో అంతర్జాతీయ కాంతి సంవత్సరంగా ్ధీన్నదన్నారు. ఇప్పటికీ పలు దేశాలు కాం లేకుండా జీవిస్తున్నాయని చెప్పారు. ప్ర తం అధికశాతంమంది విద్యార్థులు ఇంజనీ గ్ విభాగాల వైపు వెళ్తున్నారని, ఉన్న కొ ుంది అయినా పరిశోధనలు చేసి సమా నికి ఉపయోగపడాలని కోరారు. ఈ సంద ంగా ప్రొఫెసర్ మైఖేల్ పియాసెఖి ధర్మో నమిక్స్, ల్యామిని సైన్స్ వంటి అనువర్త

పరిశోధనా పత్రాల సీడీని ఆవిష్కరిస్తున్న ప్రొఫెసర్లు వీరయ్య, మైఖేల్‌పియాసెఖి తదితరులు

మానాలు గురించి వివరించారు. అలాగే ప్రొ ఫెసర్ ఎన్.వీరయ్య గ్లాస్ సైన్స్, లేజర్లు, ఎల్ ఈడీ వంటి వాటిల్లో జరుగుతున్న పరిశోధ నలు గురించి తెలిపారు. ప్రొఫెసర్లు భాస్క రన్, గాంధీలు బయోగ్లాసెస్ మీద జరుగు తున్న తమ పరిశోధన వివరాలను చెప్పారు. ముందుగా ఆంధ్ర, తెలంగాణా రాష్ట్రాల నుం చి వచ్చిన పరిశోధనా పత్రాల సీడీని వీరయ్య ఆవిష్కరించారు. ఈ సెమినార్‌కు 40 పరిశో ధనాపత్రాలు సమర్పించగా కడప, కర్నూలు, నెల్లూరు, వైజాగ్, తెలంగాణా ప్రాంతాల నుం చి 120 మంది హాజరయ్యారు. ఈ కార్యక్ర మంలో ప్రిన్సిపాల్ రాజేశ్వరి, ప్రొఫెసర్ క ల్యాణి, ఆర్గనైజింగ్ సెక్రటరీ నయూమ్, అధ్యా పకులు డాక్టర్ ఇందిర, డి.సంపూర్ణరావు తది తరులు పాల్గొన్నారు.

Dr. Md Nayeem
Dept of Physics
KRK Govt College
Addanki-523201

(A) Research publications:

S.No	***Title of the article***	***Name of the publisher// Journal with ISBN / ISSN Number***	***Year***
1.	Ultrasonic Investigations of Molecular Interaction in Binary Mixtures of Benzyl Benzoate with Isomers of Butanol	International Journal of Pharma Research & Review, Feb 2014; 3(2):65-78	2014
2.	Volumetric and viscometric study of aqueous ethylene glycol in butan-2-ol and propan-2-ol	Journal of Chemical, Biological and Physical Sciences Aug 2014 – Oct. 2014, Vol. 4, No. 4; 3092-3108; E-ISSN: 2249 –1929	2014
3.	Ultrasonic Investigations of Molecular Interaction in Binary Mixtures of Cyclohexanone with Isomers of Butanol	**Hindawi Publishing Corporation,** Journal of Applied Chemistry Volume 2014, Article ID 741795,http://dx.doi.org/10.1155/2014/741795	2014
4.	Thermoacoustic, Volumetric, and Viscometric Investigations in Binary Liquid System of Cyclohexanone with Benzyl Benzoate at T = 308.15, 313.15, and 318.15K	**Hindawi Publishing Corporation** Journal of Thermodynamics Volume 2014, Article ID 487403, http://dx.doi.org/10.1155/2014/487403	2014
5.	Ultrasonic and volumetric study of aqueous solution of ethyleneglycol, propylene glycol in iso-propanol	Journal of Chemical and Pharmaceutical Research, 2014, 6(4):1243-1258; ISSN : 0975-7384; CODEN(USA) : JCPRC5	2014
6.	Volumetric and viscometric study of aqueous solution of ethylene glycol, propylene glycol in iso-propanol	International Journal of Pharmaceutical, Chemical and Biological Sciences; IJPCBS 2014, 4(3), 691-705; ISSN: 2249-9504	2014

7.	Densities, viscosities, and excess properties for binary mixtures of ethylene glycol with amides at 308.15 K	***SPRINGER;*** Journal of Thermal Analysis and Calorimetry; DOI 10.1007/s10973-014-4019-5; ISSN 1388-6150	2014
8.	Study of some thermodynamic and acoustic properties in the solutions of acrylamide with equimolar mixture of ethanol and isopropyl alcohol/isobutyl alcohol/isoamylalcohol;	National Conference on Advanced Functional Materials and Computer Applications in Materials Technology (CAMCAT-2014) Indian Journal of Research in Pharmacy and Biotechnology ISSN: 2320-3471 (Online); 2321-5674 (Print)	2014
9.	Ultrasonic, Volumetric and Viscometric Study of Aqueous - Electrolyte Solutions	Journal of Chemical, Biological and Physical Sciences; MAY 2014 – JULY 2014, Vol. 4, No. 3; 2401-2415; E- ISSN: 2249 –1929	2014
10.	Comparative study of molecular interactions in aromatic, cyclic and aliphatic ketones with 1-octanol at 308.15 K: An insight from ultrasonic velocity and density	***ELSEVIER;*** Journal of Molecular Liquids 207 (2015) 286–293	2015
11.	Acoustic and volumetric investigations in aromatic, cyclic and aliphatic ketones with dimethyl sulphoxide at 308.15 K	***ELSEVIER;*** Arabian Journal of Chemistry, http://dx.doi.org/10.1016/j.arabjc.2015.08.005	2015
12.	Experimental and Theoretical Investigations of Ultrasonic Speed in Binary Liquid Mixtures of Benzyl Benzoate with Isomers of Butanol at T=308.15K;	Journal of Chemical and Pharmaceutical Sciences; ISSN: 0974-2115	2015
13.	Comparative analysis of molecul ar interactions between drugs of aqueous propylene glycol with certain alcohols at 308.15K: an insight from density and viscosity studies	International Journal of Pharmaceutical Sciences and Research, 2015; Vol. 6(9): 3961-3974. E-ISSN: 0975-8232; P-ISSN: 2320-5148	2015
14.	Experimental and theoretical	Journal of Chemical and	2015

	investigations of ultrasonic speed in binary liquid mixtures of ascabin with isomers of butanol at T=313.15K;	Pharmaceutical Sciences; ISSN: 0974-2115.	
15.	Thermoacoustic, volumetric, and viscometric investigations in the binary mixtures of 1,4-dioxane with n-hexane or n-heptane or n-octane	***SPRINGER;*** Journal of Thermal Analysis and Calorimetry; DOI 10.1007/s10973-015-4994-1	2015
16.	Viscometric Study of Molecular Interactions in Dimethyl Carbonate +n-Alkoxyethanol Mixtures at Different Temperatures	Journal of Thermodynamics & Catalysis; J Thermodyn Catal 2016, 7:4; DOI: 10.4172/2157-7544.1000177; ISSN: 2160-7544	2016
17.	Investigation of molecular interactions in binary mixture (benzyl benzoate + ethyl acetate) at T = (308.15, 313.15, and 318.15) K: An insight from ultrasonic speed of sound and density	***ELSEVIER;*** Journal of Molecular Liquids 218 (2016) 676–685	2016
18.	The study of solute–solvent interactions in 1-ethyl-3-methylimidazolium tetrafluoroborate + 2-ethoxyethanol from density, speed of sound, and refractive index measurements	***SPRINGER;*** Journal of Thermal Analysis and Calorimetry; DOI 10.1007/s10973-015-5205-9	2016
19.	Excess Thermodynamic Properties for Binary Mixtures of Ionic Liquid 1-Ethyl-3-methylimidazolium Ethyl Sulfate and 2-Methoxyethanol from T= (298.15 to 328.15) K at Atmospheric Pressure	***SPRINGER;*** Journal of Solution Chemistry; DOI 10.1007/s10953-016-0465-y	2016
20.	Computation of (i)activity coefficients (ii) excess chemical potential (iii) excess molar enthalpy by prigogine-flory-patterson theory for binary liquid system at T=308.15K;	National seminar GDC(A), Guntur; Full length Proceedings ISBN:978-93-85132-12-4.	2016
21.	Study of molecular interactions in binary liquid mixtures of[Emim][BF4] with 2-methoxyethanol using thermo	***ELSEVIER;*** Thermochimica Acta 630 (2016) 37–49	2016

	acoustic,volumetric and optical properties		
22.	The study of solute–solvent interactions in 1-ethyl-3-methylimidazolium ethylsulfate + 2-ethoxyethanol from density, speed of sound and refractive index measurements	***ELSEVIER;*** Journal of Molecular Liquids 218 (2016) 83–94	2016
23.	Molecular interaction studies in the binary mixture of 1-ethyl-3-methylimidazolium trifluoromethanesulphonate+1-butanol from density, speed of sound and refractive index measurements	***Taylor & Francis;*** Physics and Chemistry of Liquids ISSN: 0031-9104	2017
24.	Steric and electronic effects to interpret non-covalent interactions in binary mixtures of dimethyl carbonate and isomeric cresols through thermophysical, acoustic and spectroscopic studies	***SPRINGER;*** Journal of Thermal Analysis and Calorimetry; ISSN 1388-6150	2017
25.	Investigation of molecular interactions & prediction of calorimetric potentials of a binary liquid system at T = 308.15 K: An insight from physicochemical parameters	***ELSEVIER;*** Karbala International Journal of Modern Science, ISSN: 2405-609X	2017
26.	Investigation of solute-solvent interactions in {1-butyl-3-methylimidazoliumBis(trifluoro methylsulfonyl)imide + dimethy lcarbonate} mixture using physicochemical properties	***ELSEVIER;***The Journal of Chemical Thermodynamics; Volume 115, December 2017, Pages 133-147	2017
27.	Investigation of molecular interaction in binary system through activity coefficients and application of prigogine-flory-patterson theory to evaluate excess molar enthalpy at T=308.15K	Proceedings of the Intemational Seminar on Physics and Chemistry of Materials and Applications (ISPCMA-2017) - SPMH Kalasala, Machilipatnam. ISBN:978-93 -82570	2017
28.	Exploring molecular interactions of binary mixture (dimethyl carbonate + benzyl benzoate): Measurements and correlation	***ELSEVIER;*** Journal of Molecular Liquids; 249 (2018) 1183–1194	2017

29.	Thermophysical investigations and prediction of calorimetric potentials in binary mixture of 1-butyl-3-methylimidazolium trifluoromethanesulfonate with 1-pentanol	***SPRINGER;*** Journal of Thermal Analysis and Calorimetry;https://doi.org/ 10.1007/s10973-017-6887-y	2017
30.	A new approach- investigation of molecular interactions in binary liquid system: an insight from activity coefficients and excess chemical potentials;	National seminar Proceedings of GDC(A), Kadapa. ISBN:978-93-86251-45-9	2017
31.	Thermo-physicochemical investigation of molecular interactions in binary combination (dimethyl carbonate + methyl benzoate) Measurements and correlation	***SPRINGER;*** Journal of Thermal Analysis and Calorimetry	2017
32.	Acoustic and volumetric investigations in aromatic, cyclic and aliphatic ketones with dimethyl sulphoxide at 308.15 K	**Elsevier;** Arabian Journal of Chemistry (2019) 12, 3129–3140 http://dx.doi.org/10.1016/j.arabjc.2015.08.005	2019
33.	Binary mixtures of 2-methylcyclohexanone with various functional groups (m-cresol, p-cresol and o-chlorophenol)	**Elsevier;**Chemical Data Collections Chemical Data Collections 28 (2020) 100386 https://doi.org/10.1016/j.cdc.2020.100386	2020
34.	Computational and theoretical exploration for clinical suitability of Remdesivir drug to SARS-CoV-2	**Elsevier;**European Journal of Pharmacology; https://doi.org/10.1016/j.ejphar.2020.173642	2020
35.	A molecular interactions study between 1-butyl-3-methylimidazolium hexa-fluorophosphate ([Bmim][PF6]) and N-methylpyrrolidone	**Elsevier:** The Journal of Chemical Thermodynamics; https://doi.org/10.1016/j.jct.2020.106330	2021
36.	Target SARS-CoV-2: computation of binding energies with drugs of dexamethasone/umifenovir by molecular dynamics using OPLS-	Springer: Research on Biomedical Engineering https://doi.org/10.1007/s42600-020-00119-y	2021

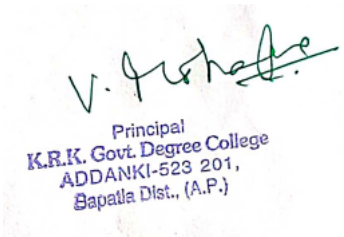
	AA force field		
37.	Target SARS-CoV-2: theoretical exploration on clinical suitability of certain drugs	Taylor & Francis: Journal of Biomolecular Structure and Dynamics https://doi.org/10.1080/07391102.2021.1924262	2021

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

(B) *Conferences/Seminars Attended*

S.No	***Title of the paper***	***Year***
1.	Study of some thermodynamic and acoustic properties in the solutions of acrylamide with equimolar mixture of ethanol and isopropylalcohol/isobutyl alcohol/isoamylalcohol; ISSN: 2320-3471.	2014
2.	Thermo-acoustical and excess thermodynamic investigations in certain ketones with DMSO at 308.15 K	2014
3.	Volumetric and Viscometric studies in aqueous Ethylene Glycol in certain alkanols	2014
4.	Experimental and theoretical investigations of ultrasonic speed in binary liquid mixtures of ascabin with isomers of butanol at T=313.15K; Journal of Chemical and Pharmaceutical Sciences; ISSN: 0974-2115.	2015
5.	Experimental and Theoretical Investigations of Ultrasonic Speed in Binary Liquid Mixtures of Benzyl Benzoate with Isomers of Butanol at T=308.15K; Journal of Chemical and Pharmaceutical Sciences; ISSN: 0974-2115	2015
6.	Computation of (i)activity coefficients (ii) excess chemical potential (iii) excess molar enthalpy by prigogine-flory-patterson theory for binary liquid system at T=308.15K; ISBN:978-93-85132-12-4.	2016
7.	Investigation of molecular interaction in binary system through activity coefficients and application of prigogine-flory-patterson theory to evaluate excess molar enthalpy at T=308.15K	2017
8.	A new approach- investigation of molecular interactions in binary liquid system: an insight from activity coefficients and excess chemical potentials; ISBN:978-93-86251-45-9	2017
9.	Rare earth phosphors – significances	2017
10.	Prediction of Density from SRK/PR Cubic EoS for a binary liquid-SRR	2017

11.	An application of computational study: Prediction of density from SRK and PR Cubic Equation of State for a binary liquid at *T=308.15K*	2017
12.	Applied Physics and Materials Science (APMS-2018)-	2018
13.	Higher Edn System in the Light of Reorganization of the states: Trends, Opportunities and Challenges	2018
14.	Fundamentals of Instrumental Analysis-Theory and Practical Training programm on NMR & HPLC-JKC	2019
15.	Recent Developments and Applications of Physico-Chemical Characterization Techniques-JKC	2019
16.		



(C) ***Invited talks delivered at Conferences / Seminars / Colleges :***

S. No	Title of the Conference / Seminar with duration	Title of the talk	Year
1.	Recent trends in Chemistry/2 days	Volumetric and Viscometric studies in aqueous Ethylene Glycol in certain alkanols	2014
2.	Recent trends in Applied Physics/2 days	Experimental and Theoretical Investigations of Ultrasonic Speed in Binary Liquid Mixtures of Benzyl Benzoate with Isomers of Butanol at T=308.15K; Journal of Chemical and Pharmaceutical Sciences; ISSN: 0974-2115	2015
3.	Awareness on Human Health/ 1 day	Got Balance?	2016
4.	Advanced trends in material science/1 day	A new approach- Investigation of molecular interactions in binary liquid system: an insight from activity coefficients and excess chemical potentials; ISBN:978-93-86251-45-9	2017

(D) Research Publications (Books, chapters in books, other than referred journal articles)

Chapter Contribution:

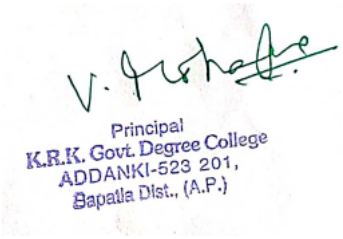
2017-18; December -Cellulose-Reinforced Nanofibre composites-	Chapter in knowledge based volumes in International publishers with ISBN numbers ***ISBN:978-0-08-100957-4***	Published by ***ELSEVIER (WP) ISBN:978-0-08-100957-4***

(E) Life member of INDIAN THERMODYNAMIC SOCIETY

(F) RC/OC/FDP/Trainings/MOOCS certificate courses completed:

S. No	Title	Place	Year
1.	Disaster Management -11-07-2016 to 30-07-2016:(108 hrs)--RC	UGC HRDC-SVU, Tirupathi	2016
2.	42 nd OC : 02-02-2015 TO 28-02-2015 ---OC	UGC-JNTUH, Hyderabad	2015
3.	Research Methodology: 20July-03 August: Ministry of Education, TLC-RC, University of Delhi--FDP	Delhi	2021
4.	Chemistry for Societal Advancements: 26-07-2021 to 31-07-2021---FDP	KLU, APKS, Amaravathi	2021
5.	Five Day e-Workshop on LaTeX-5-07-2021 to 9-07-2021	Gitam, Bangalore	2021
6.	NLW on RT & O in Physics (Online)-10-05-2021 to 17-05-2021- Workshop	VIT-AP,	2021
7.	Material Characterization Techniques--5 day FDP: 2-03-21 to 6-03-2021	Bhavan'sVivekanda College, Secunderabad	2021
8.	5 day APCCE-US FDP on New Knowledge & Energy...6-07-20 to 10-07-20	APCCE, Vijayawada	2020
9.	2 day FDP " Advances in Photonics"- 06-07-20 to 07-07-20	RGMCET, Nandyal	2020
10.	Open source Tools for Research-1 week FDP: 8-06-20 to 14-06-20	MHRD, TLC-RC, University of Delhi	2020
11.	Technology Assisted Teaching & Virtual Learning through ICT Tools--1 week International Level FDP: 25-05-20 to 30-05-20	SBVR Degree College, Badvel, Kadapa	2020
12.	SWAYAM- ARPIT :	IIT, Bombay	2020
13.	Electronic Theory of Solids: 12 week course: NPTEL	IIT, KHARAGPUR	2020
14.	Non-conventional Energy Resources: NPTEL (12 week course)	IIT, Madras	2020
15.	IYPT 2019 International Short-Term Cerificate Course	IARC/ CENTRE FOR United Nations, Mumbai	2019
16.	FDP: NPTEL-AICTE: Jul-Oct 2019 (12 weeks)	IIT Madras	2019
17.	Physics of Materials: NPTEL	IIT Madras	2019

	Certificate Course (12 week)		
18.	Nanomaterials: Experimental Design & Theoretical Modelling: 40 hr FDP	NIT Warangal, IIIT Kurnool	2021
19.	Computational Chemistry and lassical Molecular Dynamics: NPTEL: Certificate Course (8 weeks)	IIT Bombay	2018
20.	Experimental Physics-1; NPTEL (12 Weeks course)	IIT Kharagpur	2019
21	Computer Aided Drug Design to SARS-CoV-2	IIT Madras	2022



Dr. Sk. Md Nayeem

Assistant Professor of Physics,
Government Degree College, Affiliated to ANUniversity

Binary liquids
Acoustics
Volumetric
Viscometric
Thermodynamics

GET MY OWN PROFILE

	All	Since 2017
Citations	292	252
h-index	11	10
i10-index	12	10

2 articles 0 articles

not available available

Based on funding mandates

TITLE	CITED BY	YEAR
The study of solute–solvent interactions in 1-ethyl-3-methylimidazolium tetrafluoroborate+ 2-ethoxyethanol from density, speed of sound, and refractive index measurements M Srinivasa Reddy, S Nayeem, K Raju, B Hari Babu Journal of Thermal Analysis and Calorimetry 124 (2), 959-971	34	2016
Comparative study of molecular interactions in aromatic, cyclic and aliphatic ketones with 1-octanol at 308.15 K: an insight from ultrasonic velocity and density SM Nayeem, M Kondaiah, K Sreekanth, DK Rao Journal of Molecular Liquids 207, 286-293	26	2015
Thermoacoustic, Volumetric, and Viscometric Investigations in Binary Liquid System of Cyclohexanone with Benzyl Benzoate at T = 308.15, 313.15, and 318.15K DKR Sk.Md Nayeem, M. Kondaiah, K. Sreekanth Journal of Thermodynamics 2014, 13	24	2014
Excess thermodynamic properties for binary mixtures of ionic liquid 1-ethyl-3-methylimidazolium ethyl sulfate and 2-methoxyethanol from T=(298.15 to 328.15) K at atmospheric … MS Reddy, K Raju, S Nayeem, I Khan, KBM Krishana, BH Babu Journal of Solution Chemistry 45 (5), 675-701	23	2016
Investigation of molecular interactions in binary mixture (benzyl benzoate+ ethyl acetate) at T=(308.15, 313.15, and 318.15) K: An insight from ultrasonic speed of sound and … SM Nayeem, S Nyamathulla, I Khan, DK Rao Journal of Molecular Liquids 218, 676-685	20	2016
Study of molecular interactions in binary liquid mixtures of [Emim][BF4] with 2-methoxyethanol using thermo acoustic, volumetric and optical properties MS Reddy, SM Nayeem, C Soumini, KTSS Raju, BH Babu Thermochimica Acta 630, 37-49	19	2016
Densities, viscosities, and excess properties for binary mixtures of ethylene glycol with amides at 308.15 K M Kondaiah, K Sreekanth, DS Kumar, S Nayeem, DK Rao Journal of Thermal analysis and Calorimetry 118 (1), 475-483	18	2014

JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS
https://doi.org/10.1080/07391102.2021.1924262

Taylor & Francis

Target SARS-CoV-2: theoretical exploration on clinical suitability of certain drugs

Sk. Md Nayeem[a], E. Mohammed Sohail[b], N. V. Srihari[a], P. Indira[a] and M. Srinivasa Reddy[c]

[a]Department of Physics, K.R.K. Govt. Degree College, Addanki, AP, India; [b]Varinchi Super Specialty Hospital, Banjara Hills, Hyderabad, TS, India; [c]Department of Chemistry, T.R.R. Govt. Degree College, Kandukur, AP, India

Communicated by Ramaswamy H. Sarma

ABSTRACT

We propose a unique theoretical methodology because of the global high priority rating to search for the repurposed drugs that outfit clinical suitability to SARS-CoV-2. The approach is based on the exploration of structural analysis, computation of biothermodynamics, interactions and the prediction of entropy sign successively via molecular dynamics. We tested this methodology for Favipiravir/Dolutegravir drugs on the apo form of SARS-CoV-2 main protease. This theoretical exploration not only suggested the presence of strong interactions between (SARS-CoV-2 + Favipiravir/Dolutegravir) but also emphasized the clinical suitability of Favipiravir over Dolutegravir to treat SARS-CoV-2 main protease. The supremacy of Favipiravir over Doultegravir is well supported by the results of global clinical trials on SARS-CoV-2 infection. Thus, this work will pave the way for incremental advancement towards future design and development of more specific inhibitors to treat SARS-CoV-2 infection in humans.

ARTICLE HISTORY
Received 28 August 2020
Accepted 11 April 2021

KEYWORDS
Apo form of SARS-CoV-2 main protease; Favipiravir; Dolutegravir; molecular dynamics; GROMACS; biothermodynamics; entropy; interactions

1. Introduction

In recent times, myriads of people have been suffering from a novel SARS-CoV-2 (COVID-19) infection, and the death rate toll has reached thousands and been heading step by step, which is a topmost crisis across the globe (Chen, 2020). Accordingly, the demand for an investigation of the drug to forestall SARS-CoV-2 is of enormous interest for all scientific communities worldwide. The vital topic appropriate to annihilating activity of SARS-CoV-2 virus is concomitant to a variety of viruses which caused MERS (Middle East respiratory syndrome), SARS (Severe acute respiratory syndrome) (Roberts et al., 2007). These viruses, which inception the common cold in human beings over and over again. However, the new COVID-19 cause earnest evidence compared to Middle East respiratory syndrome and severe acute respiratory syndrome (Chen, 2020).

SARS-CoV-2 is a betacoronavirus, such as SARS-CoV and MERS-CoV, all of which have their beginning in chiropterans. For the aesculapian indicant, SARS-CoV-2 pathologic process reason out in fatal pneumonia with the technological provision aggravated similar to SARS-CoV-2 malady. Endure infected with COVID-19 might likewise fortify acute respiratory distress syndrome, leading to a full admittance rate to an intensive care unit and finally death in austere cases (Chen et al., 2020).

The COVID-19 virus is suited to the cysteine protease family unit. Hitherto, various business firms and scholarly people followed a line of the probe on the globe paying care on inquisitory and processing the monosemous vaccine or antiviral drug to obviate or pull off the budding pathological process of SARS-CoV-2. Conversely, such selections need much time for the developing procedure. For the imperative prerequisite to get rid of the SARS-CoV-2 virus, the use of repurposed on hand antiviral drugs is authorized to cure another viral contagion for example HIV, hepatitis B/C and influenza is to some degree anticipatory. It is based on the early action of healing after administration relevant to viruses of Middle East respiratory syndrome and severe acute respiratory syndrome (Clercq & Li, 2016; Huang et al., 2020; Liu & Wang, 2020).

As per the studies (Gralinski & Menachery, 2020; Paraskevis et al., 2020; Tipnis et al., 2000), the COVID-19 virus chooses Angiotensin-converting enzyme 2 (ACE2) of humans and from there, it gradually attacks the immune system. This enzyme is an integral casing of glycoprotein which lies in the essential issues of human beings. In this work, we used the Favipiravir/Dolutegravir drugs, which are crucial for the management of HIV. Further, the suppress activity of Favipiravir/Dolutegravir drugs on ACE2 is already proven (Tikellis & Thomas, 2012). In the present study, PDB6M03 pertinent to apo form of main protease apt to COVID-19 is the captivating drug prey for the remedy of COVID-19 pathologic process. As of late, given its positive outcomes in clinical preliminaries, Favipiravir was affirmed by the Food and Drug Administration to treat COVID-19 through emergency use authorization (Kandeel & Al-Nazawi, 2020). The structure and the source of the Protein/Drugs are shown in Table 1.

SARS-CoV-2 main protease (PDB6M03) as a drug target with certain drugs is available in the literature, but most of

CONTACT Sk. Md Nayeem mdnayeem@krkgdcaddanki.ac.in or shaikmohammadnayeem@gmail.com Department of Physics, K.R.K. Govt. Degree College, Addanki, AP 523201, India

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

European Journal of Pharmacology 890 (2021) 173642

Contents lists available at ScienceDirect

European Journal of Pharmacology

journal homepage: www.elsevier.com/locate/ejphar

Full length article

Computational and theoretical exploration for clinical suitability of Remdesivir drug to SARS-CoV-2

Shaik Mahammad Nayeem [a,*], Ershad Mohammed Sohail [b], Gajjela Priyanka Sudhir [c], Munnangi Srinivasa Reddy [d]

[a] Department of Physics, KKR Govt. Degree College, Addanki, 523201, A.P., India
[b] Virinchi Super Specialty Hospital, Banjara Hills, Hyderabad, 500034, T.S., India
[c] SGK Super Specialty Hospital, Narasaraopet, 522601, A.P., India
[d] Department of Chemistry, VRK Govt. Degree College, Kandukur, 523105, A.P., India

ARTICLE INFO

Keywords:
SARS-CoV-2 main protease
Remdesivir
Molecular dynamics
Gromacs
Gibb's free energy
Interactions
Thermodynamic potentials

ABSTRACT

A methodology for the exploration of clinical suitability of Remdesivir drug to SARS-CoV-2 main protease based on the computational, theoretical analysis pertinent to Gibb's free energy computed from the Molecular Dynamic simulations with OPLS-AA force field at 300 K/atmospheric pressure and the variation of thermodynamic potentials over the entire simulation run of 100 ns. This study emphasized the suitability of Remdesivir drug to SARS-CoV-2 protein and the same is emphasized by the results of global clinical trials. This methodology can be applied for future design, development of more specific repurposed inhibitors for the treatment of SARS-CoV-2 infection.

1. Introduction

Coronavirus disease (COVID-19) is an infection causing the severe acute respiratory syndrome. Coronavirus 2 (SARS-CoV-2), a recently revealed novel coronavirus is genetically different from viruses that trigger influenza. These are encased, single-stranded RNA viruses whose exterior is enclosed by a halo of protein spikes (corona). The SARS-CoV-2 fits in to the cysteine protease family and the fatality due to this has reached thousands and been mounting step by step, which is a major crisis in the world (Chen, 2020; Chen et al., 2020; Roberts et al., 2007). Since SARS-CoV-2 is rapidly spreading worldwide, World Health Organization (WHO) has declared it as a pandemic disease (Organization, 2020). Further, the devastation (de Wit et al., 2020; Xu et al., 2020) caused by this virus had raised high and critical interest to screen for expected medications through either sedate repurposing or novel medication advancement (Beck et al., 2020; Li and De Clercq, 2020; Lim et al., 2020; Novel, 2020; M. Wang et al., 2020). It is to be noted that the viruses need host-cell functional receptors in humans to accumulate and attack the immune system. As per the important studies (Cao et al., 2020; Gralinski and Menachery, 2020), the spike protein SARS-CoV-2 attacks the Angiotensin-converting enzyme 2 (ACE2) target protein on the surface of pulmonary epithelial cells of humans (Paraskevis et al., 2020; Tignis et al., 2020). Consequently, the challenge to search for medicines to prevent novel COVID-19 is of immense concern for all scientists around the globe. In this connection, Governments and pharmaceutical companies are paying much attention on probing and developing the unambiguous vaccine or antiviral drug to avert or manage budding infection of SARS-CoV-2. However, drug repurposing permits to quickly examine medical management, at lower costs and with diminished danger of disappointment as the wellbeing profile of the medication is commonly entrenched.

As of late, in view of its positive outcomes in clinical preliminaries, Remdesivir was affirmed by Food and Drug Administration to treat COVID-19 through emergency use authorization. With regards to Remdesivir, it is a monophosphoramidate prodrug of an adenosine simple that has an expansive antiviral range including filoviruses, paramyxoviruses, pneumoviruses, and coronaviruses (Gralinski and Menachery, 2020; Lo et al., 2017). In vitro, Remdesivir represses all human and creature corona viruses tried to date, including SARS-CoV-1 &2, (MERS)-CoV and MERS infections (Brown et al., 2019; Sheahan et al., 2020, 2017; Warren et al., 2016). Furthermore, the inhibiting action of Remdesivir drug on Ebola (Chang et al., 2020; Warren et al., 2016) and on ACE2 is already proven (Zhang and Zhou, 2020). The principal prescription experience of the recuperated patients in the US

* Corresponding author.
E-mail addresses: mdnayeem@krkgdcaddanki.ac.in, shaikmahammadnayeem@gmail.com (S.M. Nayeem).

https://doi.org/10.1016/j.ejphar.2020.173642
Received 21 July 2020; Received in revised form 2 October 2020; Accepted 8 October 2020
Available online 13 October 2020
0014-2999/© 2020 Elsevier B.V. All rights reserved.

[redacted]

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Research on Biomedical Engineering
https://doi.org/10.1007/s42600-020-00119-y

ORIGINAL ARTICLE

Target SARS-CoV-2: computation of binding energies with drugs of dexamethasone/umifenovir by molecular dynamics using OPLS-AA force field

Sk. Md Nayeem[1] · Ershad Mohammed Sohail[2] · G. Ridhima[3] · M. Srinivasa Reddy[4]

Received: 5 July 2020 / Accepted: 22 December 2020
© Sociedade Brasileira de Engenharia Biomedica 2021

Abstract

Introduction In recent times, myriads of public have been infected with a novel SARS-CoV-2, and the fatality toll has reached thousands and been mounting step by step, which is a major crisis in the world. The challenge for this burning issue pertinent to repurposed medicines which prevent novel coronavirus is of immense concern for all scientists around the globe until the arrival of the vaccine.

Methods Because of the global high priority rating on the search for the repurposed drugs which outfits clinical suitability to SARS-CoV-2, a unique theoretical methodology is proposed. The approach is based on explorations of biothermodynamics computed via molecular dynamics, root-mean-square deviation (RMSD), radius of gyration (Rg) and interactions. This unique methodology is tested for umifenovir/dexamethasone drugs on (SARS-CoV-2) main protease.

Results This theoretical exploration not only suggested the presence of strong interactions between (SARS-CoV-2 + umifenovir/dexamethasone) but also emphasized the clinical suitability of dexamethasone over umifenovir to treat SARS-CoV-2. This supremacy of dexamethasone is well supported by the results of global clinical trials and COVID-19 therapeutic approved management guidelines of countries.

Conclusions Thus, this work will pave a way for incremental advancement towards future design and development of more specific inhibitors for the treatment of SARS-CoV-2 infection in humans.

Keywords SARS-CoV-2 protein · Dexamethasone · Umifenovir · Molecular dynamics · Gromacs · Gibb's free energy · Interactions

Introduction

Coronavirus disease (COVID-19) is an infection causing the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), a recently revealed novel coronavirus. SARS-CoV-2 is genetically different from viruses that trigger influenza. These are encased, single stranded RNA viruses whose exterior is enclosed by a halo of protein spikes (corona) (Fig. 1). The SARS-CoV-2 fits into the cysteine protease family, and the fatality due to this has reached thousands and been mounting step by step, which is a major crisis in the world (Chen 2020; Roberts et al. 2007; Chen et al. 2020). Since SARS-CoV-2 is rapidly spreading worldwide, the World Health Organization (WHO) has declared it as a pandemic disease (Coronavirus disease 2019). Consequently, the challenge to search for medicines to prevent novel coronavirus is of immense concern for all scientists around the globe.

Governments and pharmaceutical companies are paying attention to probing and developing the unambiguous vaccine or anti-viral drug to avert or manage budding infection of SARS-CoV-2. On the other hand, such selections need much time for the developing procedure. Drug repurposing permits to quickly examine medical management, at lower costs and with diminished danger of disappointment as the wellbeing profile of the medication is commonly entrenched. Growing

✉ Sk. Md Nayeem
shaikmohammadnayeem@gmail.com

[1] Department of Physics, KRK Govt. Degree College, Addanki 523201, India

[2] Virinchi Super Specialty Hospital, Banjara Hills, Hyderabad 500034, India

[3] RS Clinic, 6-1-297/B/289, Gurudwara Road, Hill Colony, Vasanthalipuram, Hyderabad 500034, India

[4] Department of Chemistry, TKR Govt. Degree College, Kandukur 523105, India

Published online: 08 January 2021

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Journal of Molecular Liquids 269 (2018) 14–22

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Investigation of molecular interactions in binary liquid mixture: Measurements and correlation through thermo physicochemical study

Sk. Md Nayeem

Department of Physics, KRK Govt. Degree College, Addanki 523201, A.P., India

ARTICLE INFO

Article history:
Received 11 July 2018
Accepted 1 August 2018
Available online 04 August 2018

Keywords:
Density
Speed of sound
Extended Langmuir model
PFP theory
PR/SRK CEoS
Excess chemical potential
Derivatives of thermodynamic potentials

ABSTRACT

Density (ρ)/acoustic speed (u) of sound have been experimentally measured over the complete mole fraction on (dimethyl carbonate + diisopropyl ether) mixture at T = (308.15/313.15/318.15) K and atmospheric pressure. Investigational data have been used to gauge excess molar volume /partial molar volume/excess partial molar volume/excess values of intermolecular free length/isentropic compressibility/acoustic impedance/isobaric thermal expansion coefficient/isothermal compressibility/surface tension. Extended Langmuir model pertinent to surface tension was applied to check the depth of penetration of molecular interactions between molecules. The excess values were fitted to Redlich-Kister equation and subsequently standard deviations are evaluated from coefficients. The departures of computed excess properties were explored in terms of molecular interactions. Experimental excess molar volume in the existing adventure was correlated by *Prigogine–Flory–Patterson* (PFP) theory/*Soave-Redlich-Kwong* (SRK) CEoS/*Peng-Robinson* (PR) CEoS at 308.15 K. Theoretical excess chemical potentials are computed and correlated by *Margules/Porter/Wilson* and *VanLaar* models at 308.15 K. Furthermore, vital thermodynamical potential derivatives are worked out at all temperatures through physicochemical properties rather calorimetric experiments. Contemporary study also consists of estimation and correlation of cohesive energy ΔA, Van der Wall's constants (a, b), distance of closest approach (d) by *Hartmann–Balizar* and *Ballou* non-linear equations at all temperatures.

© 2018 Elsevier B.V. All rights reserved.

1. Introduction

With the wide range of indispensable properties, binary and multi component liquid mixtures rather than pure liquids are of great significance in several chemical, industrial and biological processes. The study and dependency of volume/acoustic properties of multi-component mixtures on concentration/temperature is a useful indicator in chemical engineering estimations [1]. Further, thermodynamics are essential for prediction of the complicated molecular interactions and mechanisms of the liquid mixtures [2]. The check of the obtainable empirical relations and the progress of new techniques for prediction of molecular interactions/derivatives of potentials, have exacting implication because they are the only way to ensure precise results and are having immense use in theoretical, practical considerations. Furthermore, the advantages of information of physicochemical parameters over calorimetric experiment in liquid systems have importance in both theoretical and investigational portions [1]. The conclusions of such study are frequently used in diverse processes of chemical and industrial sectors.

In this paper we report excess properties and derivatives of thermodynamic potentials for binary mixture of dimethyl carbonate (DMC) + diisopropyl ether (DIPE) in the temperature range from 308.15 K to 318.15 K. The liquids are selected basing on their industrial applications. Dimethyl carbonate (DMC) is an eco-friendly, low toxic chemical and used in petroleum [3]/battery science [4]. Diisopropyl ether (DIPE) is secondary ether and being used as solvent in various chemical processes. It is colorless and slightly soluble in water, but more soluble with organic solvents. It is categorized under Oxygenated compounds. It is generally added to gasoline to enhance fuel ignition competence/antiknocking property and to lower emanation of carbon monoxide/hydrocarbons.

Organized explorations of the physicochemical properties of dimethyl carbonate (DMC) with molecular organic solvents have been available in literature [5–8]. Lugo et al. [5] gauged the ρ/u in (dmc + octane) system. They derived $k_s/\alpha_p/n_i$ at (278.15–353.15) K/up to 25 MPa pressure range. Shin et al. [6] gauged ρ/refractive indices/viscosity (η) in (DMC + DPC) system. Iglesias et al. [7] measured ρ/refractive index in [DMC + Bmim][BF4]) system. Chen et al. [8] gauged $\rho/\eta/u$ at temperatures (293.15 to 333.15) K in the atmospheric pressure in (DMC + γ-GBL) system.

Methodical explorations of the physicochemical properties of diisopropyl ether (DIPE) with single or with other liquids have been reported. The authors Zhao and Jiangtao Wu [9] studied surface tension and density of diisopropyl ether from (248 to 373) K. Gonzalez-Olmos et al. [10] reported experimental data of density

E-mail address: shaikmahammadnayeem@gmail.com.

https://doi.org/10.1016/j.molliq.2018.08.003
0167-7322/© 2018 Elsevier B.V. All rights reserved.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

+ MODEL

Available online at www.sciencedirect.com

ScienceDirect

Karbala International Journal of Modern Science xx (2017) 1–9
http://www.journals.elsevier.com/karbala-international-journal-of-modern-science/

Investigation of molecular interactions & prediction of calorimetric potentials of a binary liquid system at T = 308.15 K: An insight from physicochemical parameters

Sk. Md Nayeem

Department of Physics, KRK Govt. Degree College, Addanki, 523201, A.P., India

Received 12 March 2017; revised 18 April 2017; accepted 5 May 2017

Abstract

Excess values of surface tension/isothermal compressibility/internal pressure/free volume/enthalpy/entropy and Gibbs energy are computed using the experimentally measured density (ρ) and ultrasonic speed (*u*) for the binary liquid mixtures of *dimethyl sulphoxide* with *acetophenone* at $T = 308.15$ K. Activity coefficients and excess chemical potential are estimated using Morgules, Porter, Van laar and Wilson equations. The studied system shows departure to the ideality indicating the presence of weak interactions. Further, PFP theory is tested to correlative the experimental excess molar enthalpy. Moreover, PFP theory is extended to compute different derivatives of thermodynamic potentials rather calorimetric measurements. The present investigation also encompass of assessment of the acoustic non-linearity parameter (**B/A**) along with computation of cohesive energy, **ΔA**, Van der Wall's constants (**a,b**), distance of closest approach (**d**).

© 2017 The Author. Production and hosting by Elsevier B.V. on behalf of University of Kerbala. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Keywords: Molecular interactions; PFP theory; Thermodynamic potential derivatives; Activity coefficients; Excess chemical potentials

1. Introduction

For an adequate choice of binary mixture for the possible application, the knowledge of their interaction with each other is an indispensable feature for forecasting the reactivity and selectivity. The practical application of mixed solvents rather than single solvent in biological and industrial process has been established all over the world as they provide an extensive alternative of solutions with appropriate properties [1].

It is well known fact that ultrasonic speed, density and related thermodynamic factors are helpful as well as needed for characterizing thermodynamic and physicochemical features of binary liquid mixtures for instance molecular dissociation and association. These physicochemical investigations are used to grip the mixtures of hydrocarbons etc. In the chemical industry, knowledge of the thermodynamic properties of binaries is essential in the design involving chemical separation, heat transfer, mass transfer and fluid flow. Further, the advantage of knowledge of physicochemical properties over calorimetric experiments in binary liquid mixtures has relevance in theoretical and applied

E-mail address: shaikmahammadnayeem@gmail.com.
Peer review under responsibility of University of Kerbala.

http://dx.doi.org/10.1016/j.kijoms.2017.05.001
2405-609X/© 2017 The Author. Production and hosting by Elsevier B.V. on behalf of University of Kerbala. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Please cite this article in press as: Sk. Md Nayeem, Investigation of molecular interactions & prediction of calorimetric potentials of a binary liquid system at T = 308.15 K: An insight from physicochemical parameters, Karbala International Journal of Modern Science (2017), http://dx.doi.org/10.1016/j.kijoms.2017.05.001

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Chemical Data Collections 28 (2020) 100486

Contents lists available at ScienceDirect

Chemical Data Collections

journal homepage: www.elsevier.com/locate/cdc

Binary mixtures of 2-methylcyclohexanone with various functional groups (m-cresol, p-cresol and o-chlorophenol)

Shaik Parveen Sulthana[a], Shaik Babu[b], Sk. Md. Nayeem[c], M. Gowrisankar[d,*]

[a] Department of Chemistry, Acharya Nagarjuna University, Guntur - 522510, AP, India
[b] Department of Physics, Koneru Lakshmaiah Education foundation, Vaddeswaram, AP, India
[c] Department of Physics, KRK Govt Degree college, Addanki, Prakasam District - 523201, Andhra Pradesh, India
[d] Department of Chemistry, J.K.C.C. Acharya Nagarjuna University, Guntur - 522006, AP, India

ARTICLE INFO

Article history:
Received 20 August 2019
Revised 6 March 2020
Accepted 24 March 2020
Available online 17 May 2020

Keywords:
Density
speed of sound
donor acceptor interactions
2-methylcyclohexanone
substituted phenols

ABSTRACT

The densities, speeds of sound and viscosities including those of pure liquids, were measured for the binary mixtures of 2 methylcyclohexanone with various functional groups (m-cresol, p-cresol, and o-chlorophenol) over the entire composition range at different temperatures (303.15 - 318.15) K and atmospheric pressure 0.1MPa. Using this experimentally determined data, the values of excess molar volume, excess isentropic compressibility, partial molar volumes, partial molar isentropic compressibilities and deviation in viscosity of these components at infinite dilution were calculated. The results are discussed both in terms of acid base interactions and the formation of π-π complexes between the unlike molecules. Excess molar volume values have been analyzed with Prigogine- Flory-Patterson.

© 2020 Published by Elsevier B.V.

Specifications Table

Subject Area	Physical chemistry & Chemical Thermodynamics
Compounds	2-methylcyclohexanone, m-cresol, p-cresol and o-chlorophenol
Data category	Spectral synthesized
Data acquisition format	IR
Data type	Process and analysis
Procedure	Measurements of density, viscosity, and speed of sound of above-mentioned compounds, Estimate Partial molar volumes and Partial molar Isentropic compressibilities.
Data accessibility	Data is provided with this article

1. Rationale

The Monumental features of Ionic Liquids (ILs) have a great plausible unification in contemporary epoch. Remarkably, the thermo physical distinctive features of ILs at ambient temperatures play a juggernaut role in many sectors such as industrial engineering, pharmaceutical manufacturing and waste management treatment. Hydrogen bonding between molecules of an individual component or between molecules of different components of a mixture may be treated as an extreme case of dipolar

* Corresponding author.
E-mail addresses: mail2sulthana@gmail.com (S.P. Sulthana), drshaikbabu.physics@gmail.com (S. Babu), skmdnayeem@gmail.com (Sk. Md. Nayeem), gowrisankar127@gmail.com, gowrisankar86@gmail.com (M. Gowrisankar).

https://doi.org/10.1016/j.cdc.2020.100486
2405- 8300/© 2020 Published by Elsevier B.V.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Journal of Molecular Liquids 207 (2015) 286–293

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Comparative study of molecular interactions in aromatic, cyclic and aliphatic ketones with 1-octanol at 308.15 K: An insight from ultrasonic velocity and density

Sk. Md. Nayeem [a], M. Kondaiah [b], K. Sreekanth [c], D.Krishna Rao [d,*]

[a] Department of Physics, KRK Govt. Degree College, Addanki, 523201 A.P., India
[b] Department of Physics, NM Govt. Degree College, Jegipet, 502270 Telangana, India
[c] Department of Physics, PBN College, Nidubrolu, 522124 A.P., India
[d] Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar, 522510 A.P., India

ARTICLE INFO

Article history:
Received 7 January 2015
Accepted 24 March 2015
Available online 31 March 2015

Keywords:
Ultrasonic velocity
Density
Excess properties
Redlich-Kister type polynomial
Partial molar volumes
Partial molar compressibilities
Theoretical velocity models

ABSTRACT

Ultrasonic velocities, u, densities, ρ, of binary liquid mixtures of 1-octanol with acetophenone (AP), cyclopentanone (CP), and 3-Pentanone (3P), including pure liquids, over the entire composition range have been measured at 308.15 K. Using the experimental results, parameters such as molar volume (V_m), isentropic compressibility (k_s), acoustic impedance (z) and their excess/deviation properties have been calculated. The calculated deviation/excess properties have been fitted to the Redlich–Kister type polynomial equation. Partial molar volumes, excess partial molar volumes and partial molar compressibilities, excess partial molar compressibilities have also been calculated. The observed positive values of V_m^E, Δk_s, and negative values of z^E for all the liquid mixtures indicate the domination of rupture of existing H-bond or reduction in H-bond strength between the carbonyl group (–C=O) of ketones and the hydroxyl group (–OH) of 1-octanol. The strength of weak interactions follows the order: (1-octanol + 3P) > (1-octanol + CP) > (1-octanol + AP). Further, FTIR spectra also support the conclusions drawn from excess/deviation properties. Moreover, theoretical values of sound velocity in the mixtures have been evaluated using various theories and compared with experimental sound velocities to verify the applicability of such theories to the systems studied.

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Ultrasonic velocities, densities and derived thermodynamic, acoustical parameters are of considerable interest in understanding the intermolecular interactions in binary as well as ternary liquid mixtures [1–5]. Ultrasonic studies can also be used to determine the extent of complexation and to calculate the formation constant values of charge transfer complexes [6,7]. It is well known that alcohols are highly associated through hydrogen bonds, thus their structure and properties are determined mainly by quasi-chemical bonds between the molecules which result in the formation of multimers of different sizes and structures [8]. The practical application of mixed solvents rather than single solvent in industrial and biological processes has been recognized all over the world as they provide a wide choice of solutions with appropriate properties [9]. Ketones are organic compounds that contain a carbonyl group ($>C^{+}{=}O^{-}$) and two aliphatic or aromatic substituents containing the chemical formula $RCOR^1$. Here, R and R^1 may be the same or different incorporated into a ring (alkyl, aryl and heterocyclic radicals). The chemical reactivity of the carbonyl group plays a vital role in chemical reactions and is influenced considerably by steric effects. The greater electro negativity of O^-, high dipole moment makes ketones polar. The following resonance structure (structure (a)) illustrates this polarity. Further the presence of oxygen with its non-bonding electron pairs makes them H-bond acceptors. The common solvent chosen here is 1-octanol, a straight chain fatty alcohol with eight carbon atoms (structure (b)). Chemically it is a non-polar liquid. It is used in vinyl resins, plastics, oils, and perfumes, as a defoaming agent and medicinally it is used for controlling essential tremors and other types of involuntary neurological tremors [10].

* Corresponding author.
E-mail address: krdhanekula@yahoo.co.in (D.K Rao).

http://dx.doi.org/10.1016/j.molliq.2015.03.041
0167-7322/© 2015 Elsevier B.V. All rights reserved.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

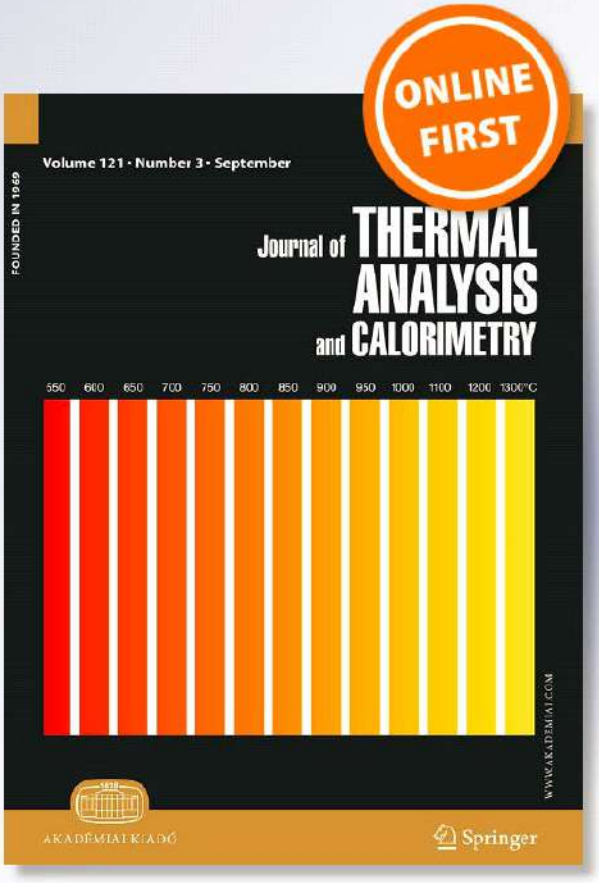
Thermoacoustic, volumetric, and viscometric investigations in the binary mixtures of 1,4-dioxane with n*-hexane or* n*-heptane or* n*-octane*

Sk. Md Nayeem, M. Kondaiah, K. Sreekanth, M. Srinivasa Reddy & D. Krishna Rao

Journal of Thermal Analysis and Calorimetry
An International Forum for Thermal Studies

ISSN 1388-6150

J Therm Anal Calorim
DOI 10.1007/s10973-015-4994-1



Springer

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Arabian Journal of Chemistry (2015) xxx, xxx–xxx

King Saud University

Arabian Journal of Chemistry

www.ksu.edu.sa
www.sciencedirect.com

REVIEW

Acoustic and volumetric investigations in aromatic, cyclic and aliphatic ketones with dimethyl sulphoxide at 308.15 K

Sk.Md Nayeem [a,*], M. Kondaiah [b], K. Sreekanth [c], D. Krishna Rao [d]

[a] Department of Physics, KRK Govt. Degree College, Addanki 523201, A.P., India
[b] Department of Physics, NM Govt. Degree College, Jogipet 502270, Telangana, India
[c] Department of Physics, PBN College, Nidubrolu 522124, A.P., India
[d] Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar, 522 510, A.P., India

Received 10 April 2015; accepted 5 August 2015

KEYWORDS

Ultrasonic velocity;
Density;
Excess properties;
Redlich–Kister type polynomial;
Theoretical velocity models

Abstract Ultrasonic velocities, u, and densities, ρ, of binary liquid mixtures of dimethyl sulphoxide (DMSO) with ketones such as acetophenone (AP), cyclohexanone (CH), and 3-pentanone (3P), including pure liquids, over the entire composition range have been measured at 308.15 K. Using the experimental data, deviation in ultrasonic velocity, Δu, deviation in isentropic compressibility, Δk_s, excess molar volume, V_m^E, excess intermolecular free length, L_f^E and excess acoustic impedance, Z^E, partial molar volumes, $\overline{V}_{m,1}$, $\overline{V}_{m,2}$, and excess partial molar volumes, $\overline{V}_{m,1}^E$, $\overline{V}_{m,2}^E$ have been calculated. Molecular interactions in the systems have been studied in the light of variation of excess/deviation values of calculated properties and these properties have been fitted to Redlich–Kister type polynomial equation. The observed positive values of V_m^E, Δk_s, L_f^E and negative values of Δu, Z^E for all the binary liquid mixtures studied clearly indicate the presence of the dominance of weak physical interactions between the components of molecules. Further, FTIR spectra support the conclusions drawn from deviation/excess properties. Moreover, theoretical values of ultrasonic velocity in the mixtures have been evaluated using various theories and such values were compared with experimental velocities to verify the applicability of such theories to the systems investigated.
© 2015 The Authors. Production and hosting by Elsevier B.V. on behalf of King Saud University. This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

* Corresponding author. Tel.: +91 863 2354395 (R), +91 9440712142.
E-mail address: krdhanekula@yahoo.co.in (S. Nayeem).
Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

http://dx.doi.org/10.1016/j.arabjc.2015.08.005
1878-5352 © 2015 The Authors. Production and hosting by Elsevier B.V. on behalf of King Saud University.
This is an open access article under the CC BY-NC-ND license (http://creativecommons.org/licenses/by-nc-nd/4.0/).

Please cite this article in press as: Nayeem, S.M. et al., Acoustic and volumetric investigations in aromatic, cyclic and aliphatic ketones with dimethyl sulphoxide at 308.15 K. Arabian Journal of Chemistry (2015), http://dx.doi.org/10.1016/j.arabjc.2015.08.005

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

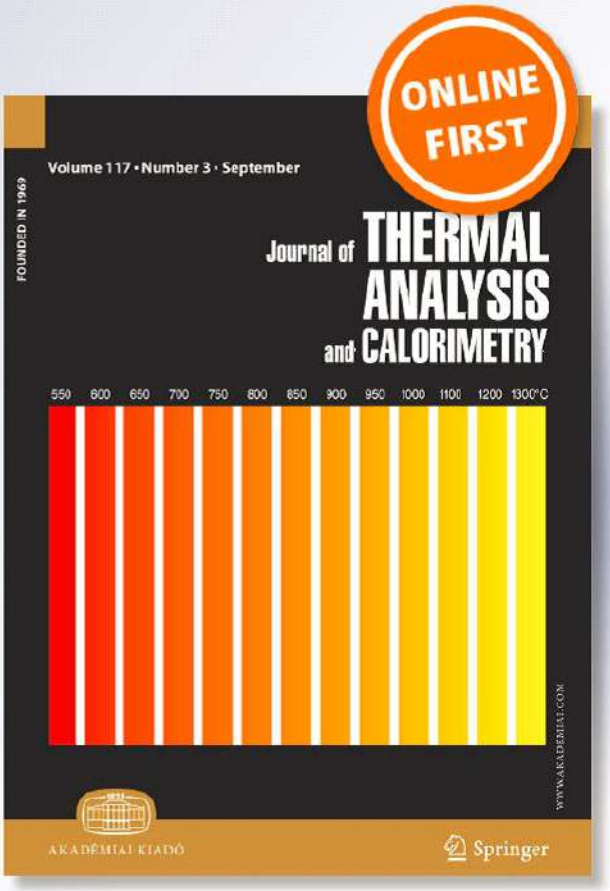
Densities, viscosities, and excess properties for binary mixtures of ethylene glycol with amides at 308.15 K

M. Kondaiah, K. Sreekanth, D. Sravana Kumar, Sk. Md. Nayeem & D. Krishna Rao

Journal of Thermal Analysis and Calorimetry
An International Forum for Thermal Studies

ISSN 1388-6150

J Therm Anal Calorim
DOI 10.1007/s10973-014-4019-5



Springer

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Journal of Molecular Liquids 218 (2016) 676–685

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Investigation of molecular interactions in binary mixture (benzyl benzoate + ethyl acetate) at $T = (308.15, 313.15, \text{and } 318.15)$ K: An insight from ultrasonic speed of sound and density

Sk. Md Nayeem [a,*], Sk. Nyamathulla [b], Imran Khan [c], D. Krishna Rao [d]

[a] Department of Physics, KRK Govt. Degree College, Addanki 523201, A.P., India
[b] Department of Physics, Govt. Degree College, Naidupet 524126, A.P., India
[c] Department of Chemistry, CICECO, University of Aveiro, Aveiro 3810-193, Portugal
[d] Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar 522 510, A.P., India

ARTICLE INFO

Article history:
Received 22 January 2016
Accepted 20 February 2016
Available online xxxx

Keywords:
Speed of sound
Density
Excess properties
Partial molar volumes
Isentropic compressibility
Enthalpy
Entropy
Gibb's free energy

ABSTRACT

Speed of sound (u) and densities (ρ) of binary liquid mixtures of benzyl benzoate with ethyl acetate, including pure liquids, over the entire composition range have been measured at $T = (308.15, 313.15 \text{ and } 318.15)$ K using the experimental data such as excess molar volume (V_m^E), excess acoustic impedance (Z^E), excess intermolecular free length (L_f^E), excess available volume (V_a^E), excess surface tension (σ^E), excess coefficient of thermal expansion (α_p^E), excess isotropic compressibility, (k_T^E), excess internal pressure (π_i^E) and excess free volume (V_f^E). Also enthalpy (H^E), entropy (S^E), Gibb's free energy (G^E), partial molar volumes/partial molar compressibilities, excess partial molar volumes/excess partial molar compressibilities, partial and excess partial molar volume of the components at infinite dilution ($\overline{V}_{m,1}^{\infty}$, $\overline{V}_{m,2}^{\infty}$), ($\overline{V}_{m,1}^{E,\infty}$ and $\overline{V}_{m,2}^{E,\infty}$) and variations of $H^E/S^E/G^E$ with change in pressure at constant temperature have been evaluated. Molecular interactions in the system have been studied in the light of variation of excess values of calculated properties and these properties have been fitted to Redlich–Kister type polynomial equation. Further, Lennard–Jones potential repulsive exponent term (n) and relative association (R_A) are computed and interpreted to elucidate the molecular interactions in the liquid mixture. The present investigation also comprises evaluation of the acoustic non-linearity parameter (B/A) in the mixtures and calculation of cohesive energy ΔA, Van der Wall's constants (a, b) and distance of the closest approach (d). Moreover, speed of sound in the mixtures has been evaluated using various semi-empirical relations and such values were compared with experimental speeds to verify applicability to the systems investigated. The computational study allows a qualitative analysis of the results in terms of the individual contribution to the excess enthalpy and Gibb's energy in terms of electrostatic, van der Waals and hydrogen bonding interaction in the binary mixture.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

Speed of sound, densities and derived thermodynamic and acoustical parameters are of considerable interest in understanding the intermolecular interactions in binary as well as ternary liquid mixtures [1–5]. In chemical industry, knowledge of the thermodynamic properties of non-electrolyte solutions is essential in the design involving chemical separation, heat transfer, mass transfer and fluid flow. Ultrasonic studies can also be used to determine the extent of complexation and to calculate the formation constant values of charge transfer complexes [6,7]. Measurement of ultrasonic speed has been adequately employed in understanding the nature of molecular interaction in pure liquid and liquid mixtures. The practical application of mixed solvents rather than single solvent in industrial and biological process has been recognized all over the world as they provide a wide choice of solutions with appropriate properties [8].

The present study deals with the thermodynamic study of mixed solvent system at $T = (308.15, 313.15 \text{ and } 318.15)$ K. The liquids under investigation have been chosen on the basis of their industrial applications. These applications have greatly stimulated the need for extensive information on the thermodynamic, acoustic and transport properties of these solvents and their mixtures [9–11].

The selected components for the present study are benzyl benzoate (BB) and ethyl acetate (EA). These possess wide applicability in various food and pharmaceutical industries. Benzyl benzoate is a carboxylate ester which is used as an insect repellent, in oily injections, as an acaricide and pediculicide in veterinary hospitals. It is an effective and inexpensive topical treatment for human scabies. Behaviour of benzyl benzoate in many liquids such as aliphatic alkanes, aromatic alkenes, aliphatic alcohols, substituted benzenes, acetates, ketones and DMSO (super solvent) [12–14] has been thoroughly studied ultrasonically.

* Corresponding author.
E-mail address: shaikmahammadnayeem@gmail.com (S.M. Nayeem).

http://dx.doi.org/10.1016/j.molliq.2016.02.045
0167-7322/© 2016 Elsevier B.V. All rights reserved.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

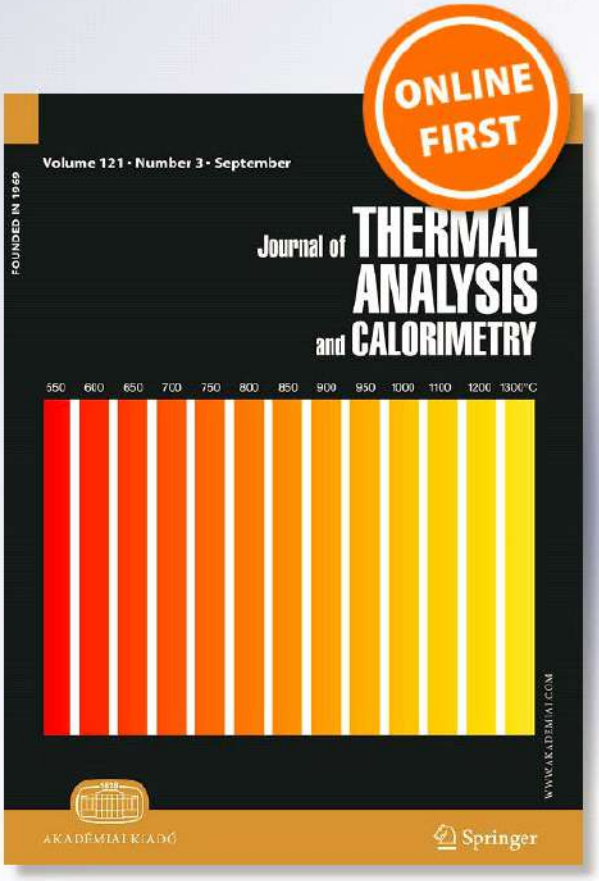
Thermoacoustic, volumetric, and viscometric investigations in the binary mixtures of 1,4-dioxane with n*-hexane or* n*-heptane or* n*-octane*

Sk. Md Nayeem, M. Kondaiah, K. Sreekanth, M. Srinivasa Reddy & D. Krishna Rao

Journal of Thermal Analysis and Calorimetry
An International Forum for Thermal Studies

ISSN 1388-6150

J Therm Anal Calorim
DOI 10.1007/s10973-015-4994-1



Springer

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

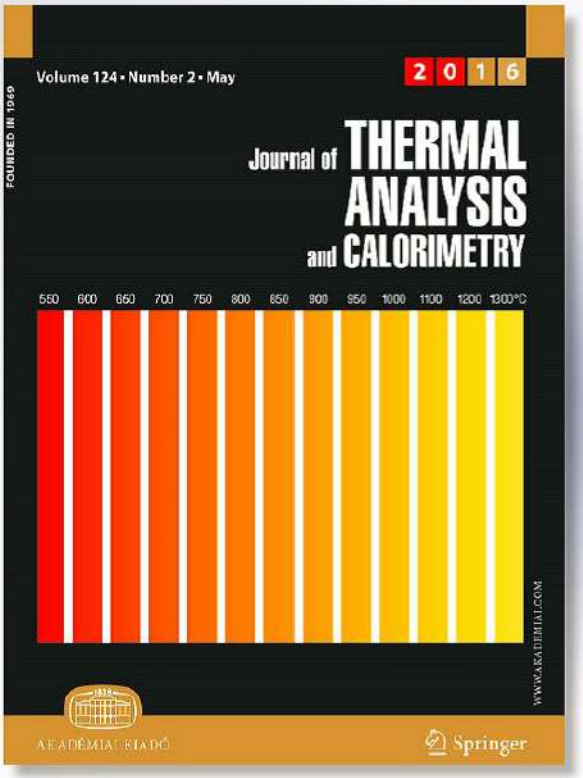
The study of solute–solvent interactions in 1-ethyl-3-methylimidazolium tetrafluoroborate + 2-ethoxyethanol from density, speed of sound, and refractive index measurements

M. Srinivasa Reddy, Sk. Md Nayeem, K. T. S. S. Raju & B. Hari Babu

Journal of Thermal Analysis and Calorimetry
An International Forum for Thermal Studies

ISSN 1388-6150
Volume 124
Number 2

J Therm Anal Calorim (2016)
124:959-971
DOI 10.1007/s10973-015-5205-9



Springer

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

MS Code : JOSL-D-15-00241 CP DISK

J Solution Chem
DOI 10.1007/s10953-016-0465-y

Excess Thermodynamic Properties for Binary Mixtures of Ionic Liquid 1-Ethyl-3-methylimidazolium Ethyl Sulfate and 2-Methoxyethanol from T = (298.15 to 328.15) K at Atmospheric Pressure

M. Srinivasa Reddy[1,5] · K. Thomas S. S. Raju[2] · Sk. Md. Nayeem[3] · Imran Khan[4,6] · K. B. M. Krishana[5] · B. Hari Babu[5]

Received: 1 October 2015 / Accepted: 23 February 2016
© Springer Science+Business Media New York 2016

Abstract The density (ρ), speed of sound (u) and refractive index (n_D) for pure [Emim][$EtSO_4$], 2-methoxyethanol and their binary mixtures were measured using an Anton Paar vibrating tube density and sound velocity meter (DSA 5000 M) and automatic refractometer over the whole composition range as a function of temperature between 298.15 and 328.15 K in steps of 10 K at atmospheric pressure. Experimental values were used to calculate the excess values of molar volumes (V_m^E), partial molar volumes ($\overline{V}_m^E$), partial molar volumes at infinite dilution ($\overline{V}_m^{E,\infty}$), isentropic compressibility (κ_S^E), acoustic impedance (Z^E), free length (L_f^E), speeds of sound (u^E), internal pressure (π_i^E), free volume (V_f^E) and deviations in refractive index ($\Delta_\phi n_D$) for the binary mixtures. These properties were fitted to a Redlich–Kister type equation to obtain the binary coefficients and the standard deviations. The negative values of V_m^E, κ_S^E, L_f^E,α_p^E,V_f^E and positive values for Z^E, u^E,π_i^E,$\Delta_\phi n_D$ indicate existence of strong interactions between the components. This was further supported by IR spectroscopy analysis.

Keywords [Emim][$EtSO_4$] · 2-Methoxyethanol · Density · Speed of sound · Refractive index · Excess/deviation parameters

✉ B. Hari Babu
dr.b.haribabu@gmail.com

[1] Department of Chemistry, KRK Govt. Degree College, Addanki, A.P. 523201, India

[2] Department of Chemistry, Andhra Loyola College, Vijayawada, A.P. 520008, India

[3] Department of Physics, KRK Govt. Degree College, Addanki, A.P. 523201, India

[4] Chemistry Department, CICECO, Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal

[5] Department of Chemistry, Acharya Nagarjuna University, N.Nagar, Guntur, A.P. 522510, India

[6] Department of Chemistry, College of Science, Sultan Qaboos University, PO Box 36, 123 Muscat, Oman

UNCORRECTED PROOF

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Thermochimica Acta 630 (2016) 37–49

Contents lists available at ScienceDirect

Thermochimica Acta

journal homepage: www.elsevier.com/locate/tca

Study of molecular interactions in binary liquid mixtures of [Emim][BF_4] with 2-methoxyethanol using thermo acoustic, volumetric and optical properties

M. Srinivasa Reddy[a,e], Sk.Md Nayeem[b], C. Soumini[c,f], K. Thomas S.S. Raju[d], B. Hari Babu[e,*]

[a] Department of Chemistry, KRK Government Degree College, Addanki 523201, A.P., India
[b] Department of Physics, KRK Government Degree College, Addanki 523201, A.P., India
[c] Department of Applied Chemistry, Cochin University of Science and Technology (CUSAT), Cochin 22, Kerala, India
[d] Department of Chemistry, Andhra Loyola College, Vijayawada 520008, A.P., India
[e] Department of Chemistry, Acharya Nagarjuna University, Nagarjunanagar 522510, A.P., India
[f] Department of Chemistry, M.E.S Ponnani College, Ponnani, Kerala, India

ARTICLE INFO

Article history:
Received 10 December 2015
Received in revised form 23 February 2016
Accepted 25 February 2016
Available online 27 February 2016

Keywords:
[Emim][BF_4]
2-Methoxyethanol
Density
Speed of sound
Refractive index
Excess/deviation thermodynamic parameters

ABSTRACT

Physical properties, such as density (ρ), speed of sound (u) and refractive index (n_D) for pure [Emim][BF_4], 2-methoxyethanol and their binary mixtures are measured over the whole composition range as a function of temperature between (298.15–328.15) K at atmospheric pressure. Experimental values were used to calculate the excess values of molar volumes (V_m^E), partial molar volumes ($\bar{V}_m^E$), partial molar volumes at infinite dilution ($\bar{V}_m^{E,\infty}$), excess/deviation values of isentropic compressibility (κ_s^E), acoustic impedance (Z^E), free length (L_f^E), speeds of sound (u^E), refractive index ($\Delta_\phi n_D$) and isobaric thermal expansion coefficient (α_p^E) for the binary mixtures. These excess/deviation properties are fitted to the Redlich–Kister type equation to obtain the binary coefficients and the standard deviations. A qualitative analysis of these parameters indicates strong intermolecular interactions between the liquids in study. This was further supported by IR spectroscopy.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

Ionic liquids (ILs) as 'green' solvents and alternative to traditional organic solvents are found increasing their utilization in many areas of technology and science such as synthesis [1,2], multiphase separations [3,4], catalysis [5–7] and as liquid electrolytes for electrochemical processes [8,9]. They consist entirely of cations and anions, with negligible vapor pressure [10], good thermal stability and broad liquid temperature ranges [11–13], non-flammability [14–18]. Organic salts that have low melting points (usually defined as below 100 °C) were collectively known as ionic liquids (ILs). The salt form and extremely low vapor pressure features garnered them much recent attention as potential solvents to replace volatile organic solvents in a wide variety of chemical reactions, separations and manufacturing processes.

Many technological processes involving ILs require the knowledge of thermo physical properties of mixing them with organic molecular solvents. To understand the interactions of their constituting cations and anions with the molecular solvents, the behavior of ILs when mixed with molecular organic solvents is of utmost importance. The IL in the investigation is [Emim][BF_4] which was widely used as solvent in organic synthesis [19,20], in biotechnology [21], in chromatography [22], etc. On the other hand, alkoxyethanols, which are amphiphilic organic solvents have been used in many chemical processes. The mixtures containing alkoxyethanols are very important from theoretical point of view, not only because of their self-association, but also due to the strong intermolecular effects produced by the presence of —O— and —OH groups in the same molecule. It is of great importance to understand the mixing behavior of ILs in alkoxyethanols and to provide accurate physicochemical data. Therefore some researchers studied the thermodynamic behavior of the mixtures of ILs with alkoxyethanols [23–26].

Systematic investigation of the physicochemical properties of [Emim][BF_4] with molecular organic solvents including water have

* Corresponding author.
E-mail address: dr.b.haribabu@gmail.com (B. Hari Babu).

http://dx.doi.org/10.1016/j.tca.2016.02.005
0040-6031/© 2016 Elsevier B.V. All rights reserved.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Journal of Molecular Liquids 218 (2016) 83–94

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

The study of solute–solvent interactions in 1-ethyl-3-methylimidazolium ethylsulfate + 2-ethoxyethanol from density, speed of sound and refractive index measurements

Srinivasa Reddy M [a,e], Md Nayeem Sk [b], Raju K.T.S.S. [c], Srinivasa Rao V [d], Hari Babu B. [e,*]

[a] Department of Chemistry, KRK Govt. Degree College, Addanki-523201, Andhra Pradesh, India
[b] Department of Physics, KRK Govt. Degree College, Addanki-523201, Andhra Pradesh, India
[c] Department of Chemistry, Andhra Loyola College, Vijayawada -520008, Andhra Pradesh, India
[d] Department of Chemistry, S.R.R&C.V.R Govt. Degree College, Vijayawada -520 004, A.P., Andhra Pradesh, India
[e] Department of Chemistry, Acharya Nagarjuna University, Nagarjunanagar-522510, Andhra Pradesh, India

ARTICLE INFO

Article history:
Received 5 November 2015
Accepted 30 January 2016
Available online xxxx

Keywords:
[Emim][$EtSO_4$]
2-ethoxyethanol
Density
Speed of sound
Refractive index
Excess/deviation parameters

ABSTRACT

Physical properties, such as density (ρ), speed of sound (u) and refractive index (n_D) for pure [Emim][$EtSO_4$], 2-ethoxyethanol and their binary mixtures are measured using Anton Paar vibrating tube density, sound velocity meter (DSA 5000 M) and automatic refract meter over the whole composition range as a function of temperature between (298.15–328.15) K at atmospheric pressure. Experimental values were used to calculate the excess molar volumes (V_m^E), excess values of partial molar volumes ($\overline{V}_m^E$), partial molar volumes at infinite dilution ($\overline{V}_m^{E,\infty}$), excess/deviation values of isentropic compressibility (κ_s^E), isothermal compressibility (κ_T^E), free length (L_f^E), speed of sound (u^E), refractive index ($\Delta_\phi n_D$), internal pressure (π_i^E), free volume (V_f^E) and isobaric thermal expansion coefficient (α_p^E) for the binary mixtures. These excess/deviation properties were fitted to the Redlich–Kister type equation to obtain the binary coefficients and the standard deviations. A qualitative analysis of these parameters indicates strong intermolecular interactions between the liquids in study. This was further supported by IR spectroscopy.

© 2015 Published by Elsevier B.V.

1. Introduction

Ionic liquids (ILs) as 'green' solvents and alternative to traditional organic solvents are found increasing their utilization in many areas of technology and science such as synthesis, catalysis, biocatalysts, electrochemical devices, separation technology, as reaction media, as green solvents and in biodegradable materials [1–9]. ILs can be chosen to have different anions and cations so that one can form IL with the desired properties. Especially, some kinds of ILs with special functional groups have been designed for application in many industrial processes. They consist entirely of cations and anions, with negligible vapor pressure [10], good thermal stability and broad liquid temperature ranges [11–13], and non-flammability [14–18]. The salt form and extremely low vapor pressure features garnered them much recent attention as potential solvents to replace volatile organic solvents in a wide variety of chemical reactions, separations, and manufacturing processes.

The potential of these new substances can be exploited with experimental methods that can reliably predict the thermodynamic properties of ionic liquids and their mixtures with other molecular solvents. Most of these novel media are characterized by their volumetric, acoustic and refractive index properties, since these data are significant for industrial applications. ILs have been considered: solvents for reactions, absorption media for CO_2 capture [19,20], the separating agent in extractive distillation [21–23], heat transfer fluids [24–26], for processing biomass [27], and the working fluid in a variety of electrochemical applications [28]. Many technological processes involving ILs require the knowledge of thermophysical properties of mixing them with organic molecular solvents. To understand the interactions of their constituting cations and anions with the molecular solvents, the behavior of ILs when mixed with molecular organic solvents is of utmost importance. The IL in the investigation, 1-ethyl-3-methylimidazolium ethyl sulfate {[Emim][$EtSO_4$]} which is used as extracting solvent for the removal of many organic compounds through liquid–liquid extraction [29,30]. It is also widely used in enzyme catalysis in ionic liquids [31], in chromatography [32], etc. On the other hand, alkoxyethanols, which are amphiphilic organic solvents have been used in many chemical processes. The mixtures containing alkoxyethanols are very important from theoretical point of view, not only of their self-association, but also due to the strong intermolecular effects produced by the presence of –O– and –OH groups in the same molecule. It is of great importance to understand the mixing behavior of ILs in alkoxyethanols and to provide accurate physicochemical data. Therefore some researchers studied the thermodynamic behavior of the mixtures of ILs with alkoxyethanols [33–

* Corresponding author.

http://dx.doi.org/10.1016/j.molliq.2016.01.096
0167-7322/© 2015 Published by Elsevier B.V.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

PHYSICS AND CHEMISTRY OF LIQUIDS, 2017
http://dx.doi.org/10.1080/00319104.2017.1279615

Taylor & Francis
Taylor & Francis Group

Molecular interaction studies in the binary mixture of 1-ethyl-3-methylimidazolium trifluoromethanesulphonate+1-butanol from density, speed of sound and refractive index measurements

M. Srinivasa Reddy[a,d], K. Thomas.S.S. Raju[b], Sk. Md Nayeem[c], K. Bala Murali Krishna[d] and Hari Babu Bollikolla[d]

[a]Department of Chemistry, KRK Govt. Degree College, Addanki, A.P., India; [b]Department of Chemistry, Andhra Loyola College, Vijayawada, A.P., India; [c]Department of Physics, KRK Govt. Degree College, Addanki, A.P., India; [d]Department of Chemistry, Acharya Nagarjuna University, Nagarjunanagar, A.P., India

ABSTRACT

A molecular interaction study was carried out between the ionic liquid 1-ethyl-3-methylimidazolium trifluoromethanesulphonate and 1-butanol using the experimental values of density, speed of sound and refractive index measurements over the whole composition range as a function of temperature between 298.15 and 328.15 K at atmospheric pressure. The excess/deviation properties such as molar volumes (V_m^E), partial molar volumes ($\bar{V}_m^E$), partial molar volumes at infinite dilution ($\bar{V}_m^{E,\infty}$), isentropic compressibility (κ_s^E), free length (L_f^E), speeds of sound (u^F), refractive index ($\Delta_\phi n_D$) and isobaric thermal expansion coefficient (a_p^E) obtained from the experimental data were fitted into the Redlich–Kister type equation to obtain the binary coefficients and the standard deviations. The excess values clearly indicated the existence of strong molecular interactions between the studied components. A quantitative analysis of these parameters was further supported by IR spectroscopic analysis. In addition, analysis of V_m^E data of the mixture was done through the Prigogine–Flory–Patterson theory.

ARTICLE HISTORY
Received 10 November 2016
Accepted 4 January 2017

KEYWORDS
[Emim][Triflate]; 1-butanol; density; speed of sound; refractive index; excess /deviation properties

1. Introduction

Ionic liquids (ILs) as substitutes for volatile organic solvents are found escalating rapidly as utilised in several areas of technology and science like an effective medium for chemical syntheses, catalysis, biodegradable materials, electrochemical devices, separation science, green solvents and biocatalysts [1–3]. Mixing of the ILs with molecular solvents is one of the alternative steps to reduce the use of ILs and to save time for synthesising new ILs. From an economic and ecological point of view, the mixtures of ILs and conventional organic solvents may be gaining a remarkable amount of attention from both the researchers and the industries. Development of the physico-chemical properties of the common ILs into the mixtures with better properties is a distinctive approach to exploit their potential applications [4]. ILs are more viscous than conventional organic solvents, which may hamper their application. Fortunately, their mixtures with molecular solvents show reduced viscosity without affecting their advantages as green solvents. In particular, the addition of polar co-solvents can strongly influence the physical and chemical properties of ILs such as viscosity, reactivity and electrical conductivity as well as solubility and solvation properties [5]. Recently, several binary IL+ molecular solvent systems have been shown to

CONTACT Hari Babu Bollikolla dr.b.haribabu@gmail.com
Supplemental data for this article can be accessed here.
© 2017 Informa UK Limited, trading as Taylor & Francis Group

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

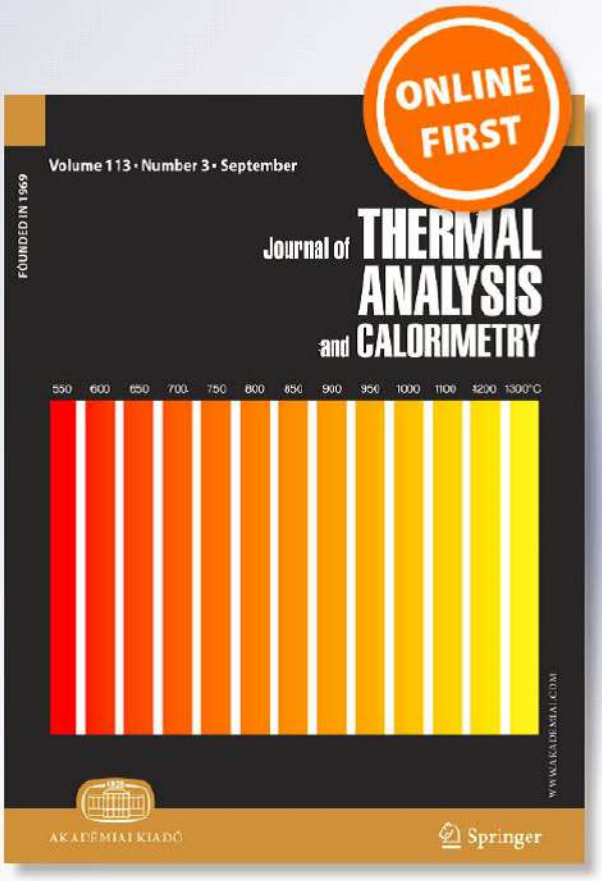
Steric and electronic effects to interpret non-covalent interactions in binary mixtures of dimethyl carbonate and isomeric cresols through thermophysical, acoustic and spectroscopic studies

Sk. Beebi, Sk. Md. Nayeem, P. B. Sandhya Sri, G. R. Satyanarayana, Zareena Begum & C. Rambabu

Journal of Thermal Analysis and Calorimetry
An International Forum for Thermal Studies

ISSN 1388-6150

J Therm Anal Calorim
DOI 10.1007/s10973-017-6225-4



Springer

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Journal of Molecular Liquids 249 (2018) 1183–1194

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Exploring molecular interactions of binary mixture (dimethyl carbonate + benzyl benzoate): Measurements and correlation

G. Jyothirmai [a], Sk. Md Nayeem [b], Imran Khan [c,d], Ch. Anjaneyulu [e,*]

[a] Department of Physics, Govt. Degree Women's College (A), Guntur 522001, AP, India
[b] Department of Physics, KRK Govt. Degree College, Addanki 523201, AP, India
[c] Department of Chemistry, College of Science, Sultan Qaboos University, Muscat, Oman
[d] CICECO-Aveiro institute of Materials, Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal
[e] Department of Physics, Bapatla Engineering College, Bapatla 522101, AP, India

ARTICLE INFO

Article history:
Received 4 November 2017
Accepted 10 November 2017
Available online 13 November 2017

Keywords:
Density
Speed of sound
Excess thermodynamic properties
Prigogine–Flory–Patterson theory
Langmuir model
Dimethyl carbonate
Benzyl benzoate

ABSTRACT

To explore the type of interaction and its behavior with temperature in the binary mixture (dimethyl carbonate + benzyl benzoate), the density (ρ) and speed of sound (u) are measured for the whole mole fraction range at various temperatures $T = (308.15, 313.15$ and $318.15)$ K and at atmospheric pressure. Sign with magnitude of computed excess molar volume (V_m^E) was examined and detailed analysis elucidated not only prevalence of strong molecular interactions between molecules in study but also its variation with temperature. Further, strong interactions are well supported by partial and their excess partial molar volume ($\overline{V}_m, \overline{V}_m^E, \overline{V}_m^{E,\infty}$). Furthermore, relative association (R_A), Lennard-Jones repulsive power (n), excess isentropic compressibility (κ_S^E), partial and their excess partial molar isentropic compressibility ($\overline{K}_m, \overline{K}_m^E$), excess values of isobaric thermal expansion coefficient (α_p^E), isentropic compressibility (κ_S^E), isothermal compressibility (k_T^E), intermolecular free length (L_f^E), acoustic impedance (Z^E), surface tension (σ_S^E), ultrasonic speed (u^E) were evaluated and confirmed the conclusions made for V_m^E. By Redlich-Kister equation, coefficients with standard deviations are computed to excess parameters. V_m^E is correlated by Prigogine–Flory–Patterson (PFP) and Topology theories at 308.15 K. Extended Langmuir model is examined for influence of the bulk mole fraction on surface tension. At $T = 308.15$ K, different derivatives of thermodynamic potentials, densities through Soave-Redlich-Kwong (SRK)/Peng-Robinson (PR) cubic equation of states, excess chemical potential and theoretical speeds using semi-empirical equations are evaluated. Using *Hartmann–Balizar* and *Ballou* non-linear equations, cohesive energy (ΔA), van der Wall's constants (a, b), distance of closest approach (d) are estimated through Sehgal's equations at all temperatures.

© 2017 Elsevier B.V. All rights reserved.

1. Introduction

The thermo-physical and acoustic properties of the pure liquids and their mixtures are investigated for numerous causes, most vital of which is to present the information concerning molecular interactions in liquid mixtures [1], which are having immense use in theoretical and practical considerations. It is well known fact that the density is essential in many chemical engineering estimations such as in designing the dimensions of boilers, condensers and storage deposits etc., [2,3]. Ultrasonic studies in liquid mixtures can be used to determine the effect of structure of donor molecules and polarity of medium on the stability of complexes which play a significant role in complexation [4] and formation constant values of charge transfer complexes to compare their stabilities [5]. With the wide range of requisite properties, binary and multiconstituent liquid mixtures sooner than pure fluids are of immense significance in numerous chemical, engineering and biological processes [6]. Further, information of the reliance of density/speed of sound on the composition, temperature and pressure is imperative in realizing the intermolecular interfaces and phase behavior of liquids. Furthermore, numerous parameters are possible to predict with density, speed of sound (physicochemical properties) and it show its bang which goes from underwater acoustics to natural science and pharmaceuticals. Thus, physicochemical parameters play vital role in calculating nano to macro level characteristic properties significant to binary liquid in study.

The liquid solvents in the present system are chosen based on their industrial and medicinal importance. Dimethyl carbonate (DMC) a biodegradable chemical as a consequence of this it frequently pondered to be a green solvent, used as an alternative of methyl *tert*-butyl ether in fuels [7]/in lithium battery technology [8], it is a strong contender in gasoline industry due to its high oxygen content (octane enhancing capacity), and it has low toxicity [9,10]. Benzyl benzoate (BB) is a carboxylate ester which is utilised as insect disgusting/in greasy injections/as a

* Corresponding author.
E-mail addresses: chanjaneyulu9@gmail.com, bec_principal@yahoo.com (C. Anjaneyulu).

https://doi.org/10.1016/j.molliq.2017.11.070
0167-7322/© 2017 Elsevier B.V. All rights reserved.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Journal of Thermal Analysis and Calorimetry
https://doi.org/10.1007/s10973-017-6887-y

Thermophysical investigations and prediction of calorimetric potentials in binary mixture of 1-butyl-3-methylimidazolium trifluoromethanesulfonate with 1-pentanol

M. SrinivasaReddy[1,5] · G. Srinivasa Rao[2] · SK. Md Nayeem[3] · K. T. S. S. Raju[4] · B. Hari Babu[5]

Received: 19 July 2017 / Accepted: 3 December 2017
© Akadémiai Kiadó, Budapest, Hungary 2017

Abstract

Physical properties, such as density (ρ) and speed of sound (u) of [Bmim][triflate], 1-pentanol and their binary mixtures, are measured over the whole composition range as a function of temperature between 298.15 and 328.15 K at atmospheric pressure. Experimental values are used to calculate the excess molar volumes (V_m^E), excess values of partial molar volumes ($\overline{V}_m^E$), partial molar volumes at infinite dilution ($\overline{V}_m^{E,\infty}$), excess values of isentropic compressibility (κ_s^E), free length (L_f^E), speeds of sound (u^E) and isobaric thermal expansion coefficient (σ_P^E) for the binary mixture. These excess properties are fitted to the Redlich–Kister-type equation to obtain the binary coefficients and the standard deviations. A qualitative analysis of these parameters indicates strong intermolecular interactions in both the systems and the interaction increases with the increase in temperature. An attempt has been made to predict derivatives of thermodynamic potentials through physicochemical parameters, and using empirical relations excess chemical potentials/molecular properties of the mixtures from nonlinear parameter are also computed at 308.15 K. The presence of strong interactions was further supported by IR spectroscopy. In addition, analysis of V_m^E data of the mixture was done through the Prigogine–Flory–Patterson theory.

Keywords [Bmim][triflate] · 1-Pentanol · Density · Speed of sound · Excess thermodynamic parameters

Introduction

Ionic liquids (ILs) as 'green' solvents represent a class of liquid materials with unique properties and alternative to traditional volatile organic solvents. Their applications are escalating rapidly as utilized in several areas of technology and science [1–3]. Mixing of the ionic liquids with molecular solvents is one of the alternative steps to reduce the use of expensive ionic liquids and to save time for synthesizing new ionic liquids of desired properties. The mixtures of ionic liquids and conventional organic solvents may be gaining a remarkable amount of attention from both the researchers and industries from both economic and ecological points of view. Improvement in the physicochemical properties of the common ILs into their mixtures with molecular organic solvents is a distinctive approach to exploit their potential applications [4]. High viscosity of ILs may hamper their industrial and research applications. Fortunately, their mixtures with molecular solvents show reduced viscosity without affecting their advantages as green solvents. In particular, the addition of polar co-solvents can strongly influence the physical and chemical properties of ILs such as viscosity, reactivity and electrical conductivity as well as solubility and solvation properties [5]. Recently, several binary IL + molecular solvent systems have been shown to perform better than the pure ILs,

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s10973-017-6887-y) contains supplementary material, which is available to authorized users.

✉ B. Hari Babu
dr.b.haribabu@gmail.com

1 Department of Chemistry, TRR Govt. Degree College, Kandukur, AP 523105, India

2 Department of Mathematics, QIS College of Engineering and Technology, Ongole, AP 523001, India

3 Department of Physics, KRK Govt. Degree College, Addanki, AP 523201, India

4 Department of Chemistry, Andhra Loyola College, Vijayawada, AP 520008, India

5 Department of Chemistry, Acharya Nagarjuna University, Nagarjuna Nagar, AP 522510, India

Published online: 15 December 2017

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Journal of Thermal Analysis and Calorimetry
https://doi.org/10.1007/s10973-017-6926-8

Thermo-physicochemical investigation of molecular interactions in binary combination (dimethyl carbonate + methyl benzoate)

Measurements and correlation

G. Jyothirmai[1] · Sk. Md. Nayeem[2] · Imran Khan[3,4] · Ch. Anjaneyulu[5]

Received: 20 November 2017 / Accepted: 11 December 2017
© Akadémiai Kiadó, Budapest, Hungary 2017

Abstract

To probe the nature of interaction and its deeds with temperature in the binary combination (dimethyl carbonate + methyl benzoate), the density (ρ)/speed of sound (u) be established for the total mole fraction array at $T = (308.15, 313.15$ and $318.15)$ K and at atmospheric pressure. Sign with magnitude of evaluated excess molar volume (V_m^E) was inspected and comprehensive analysis elucidated not only pervasiveness of strong molecular interactions between molecules but also its transform with temperature. Additional, strong interactions are properly hold up by partial and excess partial molar volume ($\overline{V}_m$, $\overline{V}_m^E$, $\overline{V}_m^{E,\infty}$). Additionally, relative association (R_A), Lennard-Jones repulsive power (n), excess isentropic compressibility (κ_s^E), partial and their excess partial molar isentropic compressibility ($\overline{K}_m$, $\overline{K}_m^E$), excess values of isobaric thermal expansion coefficient (α_P^E), isothermal compressibility (k_T^E), intermolecular free length (L_f^E), acoustic impedance (Z^E), ultrasonic speed (u^E) were evaluated and confirmed the deductions of V_m^E. By Redlich–Kister equation, standard deviations are computed through coefficients for excess parameters. At $T = 308.15$ K, V_m^E is correlated by theories of Prigogine–Flory–Patterson (PFP)/topology/Soave–Redlich–Kwong (SRK)/Peng–Robinson (PR) cubic equation of states; prophesied first-order derivatives of thermodynamic potentials; using semi-empirical equations, excess chemical potential/activity coefficients/theoretical speeds are estimated and correlated. Further, microscopic molecular properties are assessed at all temperatures by Sehgal's equations on nonlinear relations.

Keywords Density · Sound speed · Excess parameters · Prigogine–Flory–Patterson theory · Theory of topology · SRK/PR EoS · Activity coefficients · Nonlinear equations

Introduction

The thermo-physicochemical properties of the fluid and their combinations are explored for several reasons, mainly to predict the knowledge pertaining to molecular interactions in liquid amalgamation [1], which comprise enormous employ in theoretical and applied sciences. It is accurately accepted information that the volumetric property is crucial in numerous manufacturing industries in assessments such as in modelling the magnitudes of boilers, condensers and storage deposits etc., [2, 3]. Acoustic examination in liquid blend can be used to ascertain the consequence of arrangement of donor constituents and

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s10973-017-6926-8) contains supplementary material, which is available to authorized users.

✉ Ch. Anjaneyulu
chanjaneyulu9@gmail.com

[1] Department of Physics, Govt. Degree Women's College (A), Guntur, A.P. 522001, India

[2] Department of Physics, KRK Govt. Degree College, Addanki, A.P. 523201, India

[3] Department of Chemistry, College of Science, Sultan Qaboos University, Muscat, Oman

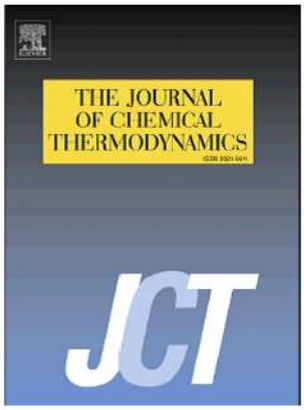
[4] Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal

[5] Department of Physics, Bapatla Engineering College, Bapatla, A.P. 522101, India

Published online: 22 December 2017

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Accepted Manuscript



Investigation of solute-solvent interactions in {1-butyl-3-methyl imidazolium-Bis(trifluoromethylsulfonyl)imide+dimethylcarbonate} mixture using physico-chemical properties

V. Srinivasa Rao, M. Srinivasa Reddy, Sk. MdNayeem, K. Thomas S.S. Raju, K. Bala Murali Krishna, B. Hari Babu

PII: S0021-9614(17)30238-0
DOI: http://dx.doi.org/10.1016/j.jct.2017.07.013
Reference: YJCHT 5131

To appear in: *J. Chem. Thermodynamics*

Received Date: 25 April 2017
Revised Date: 20 June 2017
Accepted Date: 6 July 2017

Please cite this article as: V. Srinivasa Rao, M. Srinivasa Reddy, Sk. MdNayeem, K.T.S.S. Raju, K. Bala Murali Krishna, B. Hari Babu, Investigation of solute-solvent interactions in {1-butyl-3-methyl imidazoliumBis(trifluoromethylsulfonyl)imide+dimethylcarbonate} mixture using physicochemical properties, *J. Chem. Thermodynamics* (2017), doi: http://dx.doi.org/10.1016/j.jct.2017.07.013

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Journal of Thermal Analysis and Calorimetry
https://doi.org/10.1007/s10973-018-7574-3

Investigation of molecular interactions in binary mixture of dimethyl carbonate + *N*-methylformamide at T = (303.15, 308.15, 313.15 and 318.15) K

Thermo-physical and spectroscopic study

Sk. Beebi[1] · Sk. Md. Nayeem[2] · C. Rambabu[3]

Received: 26 December 2017 / Accepted: 19 July 2018
© Akadémiai Kiadó, Budapest, Hungary 2018

Abstract
Density (ρ) and speed of sound (u) of binary liquid mixtures of dimethyl carbonate and *N*-methylformamide have been determined at T = (303.15, 308.15, 313.15 and 318.15) K over the entire composition range. Experimental data are used to evaluate excess values of molar volume (V_m^E), isentropic compressibility (k_s^E), isothermal compressibility (k_T^E), intermolecular free length (L_f^E), acoustic impedance (Z^E) and ultrasonic speed (u^E). The V^E data in the present investigation were analysed by using Prigogine–Flory–Patterson (PFP) theory. Partial and excess partial molar volumes ($\bar{V}_{m,1}$, $\bar{V}_{m,2}$), ($V_{m,1}^E$, $\bar{V}_{m,2}^E$) and partial and excess partial molar volume of the components at infinite dilution ($\overline{V}_{m,1}^{\infty}$, $\overline{V}_{m,2}^{\infty}$), ($\overline{V}_{m,1}^{E,\infty}$, $\overline{V}_{m,2}^{E,\infty}$) at T = (303.15, 308.15, 313.15, 318.15) K have been calculated. The excess/deviation properties were fitted to Redlich–Kister equation to obtain their coefficients and standard deviations. The present investigation also comprises the acoustic non-linearity parameter (B/A) in the mixtures and calculation of cohesive energy ΔA, Van der Wall's constants (a, b) and distance of closest approach (d). Moreover, various semi-empirical relations of ultrasonic speed have been used to correlate the theoretical velocities. FT-IR spectra of pure components and their binaries have been measured at T = 298.15 K.

Keywords Excess molar volume · Partial molar volumes · Isentropic compressibility · PFP theory · FT-IR spectra

Introduction

The thermo-physical properties of pure liquids and liquid mixtures are studied for many reasons, most important of which is to provide information about molecular interactions in liquid mixtures [1], which are having immense use in theoretical and practical considerations. In practical aspect, the density is necessary in lot of chemical engineering calculations such as in designing the dimensions of boilers, condensers and storage deposits, etc. [2, 3]. Ultrasonic studies of liquid mixtures can be used to determine the effect of structure of donor molecules and polarity of medium on the stability of complexes which play a significant role in complexation [4] and formation of constant values of charge transfer complexes to compare their stabilities [5]. With the wide range of requisite properties, binary and multi-component liquid mixtures rather than pure liquids are of great importance in several chemical, industrial and biological processes [6].

The liquids in the present system are chosen based on their industrial importance. Dimethyl carbonate (DMC) is a benign biodegradable chemical that it is investigated as substitute of methyl *tert*-butyl ether in fuels [7]. DMC has

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s10973-018-7574-3) contains supplementary material, which is available to authorised users.

✉ Sk. Beebi
beebishaik99@gmail.com

[1] Department of Chemistry, Y.V.N.R. Govt. Degree College, Kaikaluru, A.P 521333, India

[2] Department of Physics, KRK Govt. Degree College, Addanki, A.P 523201, India

[3] Department of Chemistry, Acharya Nagarjuna University, Guntur, A.P 522510, India

Published online: 16 August 2018

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Journal of Thermal Analysis and Calorimetry
https://doi.org/10.1007/s10973-017-6887-y

Thermophysical investigations and prediction of calorimetric potentials in binary mixture of 1-butyl-3-methylimidazolium trifluoromethanesulfonate with 1-pentanol

M. SrinivasaReddy[1,5] · G. Srinivasa Rao[2] · SK. Md Nayeem[3] · K. T. S. S. Raju[4] · B. Hari Babu[5]

Received: 19 July 2017 / Accepted: 3 December 2017
© Akadémiai Kiadó, Budapest, Hungary 2017

Abstract

Physical properties, such as density (ρ) and speed of sound (u) of [Bmim][triflate], 1-pentanol and their binary mixtures, are measured over the whole composition range as a function of temperature between 298.15 and 328.15 K at atmospheric pressure. Experimental values are used to calculate the excess molar volumes (V_m^E), excess values of partial molar volumes ($\overline{V}_m^E$), partial molar volumes at infinite dilution ($\overline{V}_m^{E,\infty}$), excess values of isentropic compressibility (κ_s^E), free length (L_f^E), speeds of sound (u^E) and isobaric thermal expansion coefficient (α_p^E) for the binary mixture. These excess properties are fitted to the Redlich–Kister-type equation to obtain the binary coefficients and the standard deviations. A qualitative analysis of these parameters indicates strong intermolecular interactions in both the systems and the interaction increases with the increase in temperature. An attempt has been made to predict derivatives of thermodynamic potentials through physicochemical parameters, and using empirical relations excess chemical potentials/molecular properties of the mixtures from nonlinear parameter are also computed at 308.15 K. The presence of strong interactions was further supported by IR spectroscopy. In addition, analysis of V_m^E data of the mixture was done through the Prigogine–Flory–Patterson theory.

Keywords [Bmim][triflate] · 1-Pentanol · Density · Speed of sound · Excess thermodynamic parameters

Introduction

Ionic liquids (ILs) as 'green' solvents represent a class of liquid materials with unique properties and alternative to traditional volatile organic solvents. Their applications are escalating rapidly as utilized in several areas of technology and science [1–3]. Mixing of the ionic liquids with molecular solvents is one of the alternative steps to reduce the use of expensive ionic liquids and to save time for synthesizing new ionic liquids of desired properties. The mixtures of ionic liquids and conventional organic solvents may be gaining a remarkable amount of attention from both the researchers and industries from both economic and ecological points of view. Improvement in the physicochemical properties of the common ILs into their mixtures with molecular organic solvents is a distinctive approach to exploit their potential applications [4]. High viscosity of ILs may hamper their industrial and research applications. Fortunately, their mixtures with molecular solvents show reduced viscosity without affecting their advantages as green solvents. In particular, the addition of polar co-solvents can strongly influence the physical and chemical properties of ILs such as viscosity, reactivity and electrical conductivity as well as solubility and solvation properties [5]. Recently, several binary IL + molecular solvent systems have been shown to perform better than the pure ILs,

Electronic supplementary material The online version of this article (https://doi.org/10.1007/s10973-017-6887-y) contains supplementary material, which is available to authorized users.

✉ B. Hari Babu
dr.b.haribabu@gmail.com

1 Department of Chemistry, TRR Govt. Degree College, Kandukur, AP 523105, India

2 Department of Mathematics, QIS College of Engineering and Technology, Ongole, AP 523001, India

3 Department of Physics, KRK Govt. Degree College, Addanki, AP 523201, India

4 Department of Chemistry, Andhra Loyola College, Vijayawada, AP 520008, India

5 Department of Chemistry, Acharya Nagarjuna University, Nagarjuna Nagar, AP 522510, India

Published online: 15 December 2017

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Hindawi Publishing Corporation
Journal of Applied Chemistry
Volume 2014, Article ID 741795, 11 pages
http://dx.doi.org/10.1155/2014/741795

Research Article

Ultrasonic Investigations of Molecular Interaction in Binary Mixtures of Cyclohexanone with Isomers of Butanol

Sk. Md Nayeem,[1] M. Kondaiah,[2] K. Sreekanth,[3] and D. Krishna Rao[4]

[1]*Department of Physics, KRK Government Degree College, Addanki 523 201, India*
[2]*Department of Physics, NM Government Degree College, Jogipet, Medak District, Telangana, India*
[3]*Department of Physics, PBN College, Nidubrolu, Guntur District, India*
[4]*Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar 522 510, India*

Correspondence should be addressed to D. Krishna Rao; krdhanekula@yahoo.co.in

Received 11 August 2014; Revised 21 October 2014; Accepted 3 November 2014; Published 18 December 2014

Academic Editor: Parsotam H. Parsania

Copyright © 2014 Sk. Md Nayeem et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

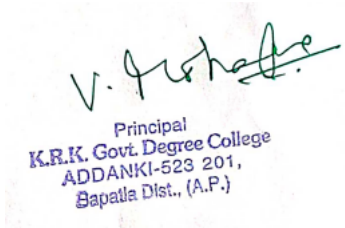
Ultrasonic speed, u, and density, ρ, have been measured in binary liquid mixtures of cyclohexanone with the isomers of butanol (*n*-butanol, *sec*-butanol, and *tert*-butanol) at 308.15 K over the entire range of composition. Molar volume (V_m), adiabatic compressibility (k_s), intermolecular free length (L_f), acoustic impedance (z), and their excess/deviation along with Δu have been calculated from the experimental data. These values have been fitted to Redlich-Kister type polynomial equation. Positive values of V_m^E, Δk_s, L_f^E and negative values of z^E, Δu have been observed for all the liquid mixtures indicating the existence of weak interactions between components. Rupture of H-bond or reduction in H-bond strength of isomers of butanol or breaking of the structure of one or both of the components in a solution causes the existence of dispersions in the present investigated binary mixtures. The data obtained from $\overline{V}_{m,1}$, $\overline{V}_{m,2}$, and excess partial molar volumes $\overline{V}_{m,1}^E$, $\overline{V}_{m,2}^E$, reflects the inferences drawn from V_m^E. Furthermore, FTIR spectra support the conclusions drawn from excess/deviation properties. The measured values of ultrasonic speed for all the investigated mixtures have been compared with the theoretically estimated values using empirical relations such as, Nomoto, Van Dael and Vangeels, Impedance and Rao specific sound speed.

1. Introduction

Ultrasonic measurements are very useful in chemical and food processing, pharmaceuticals, material testing, and underwater ranging and cleaning and are also commonly employed in mechanical machinery of materials [1], preparation of colloids or emulsions, the pregermination of seeds, imaging of biological tissues [2], activation energy of metabolic process [3], formation and destruction of azeotropes in petrochemical industries [4], and nondestructive testing (NDT).

Alcohols are self-associated organic liquids, used for the synthesis of other organic compounds. They are also widely used as coupling and dispersing agents in the chemical, pharmaceutical, and household industries and as carrier and extraction solvents for natural products. Cyclohexanone and its derivatives are used for the synthesis of pharmaceuticals, dyes, herbicides, pesticides, plasticizers, and rubber chemicals. Ketones are a class of an organic compound that contains a carbonyl group and two aliphatic or aromatic substituents containing the chemical formula RCOR[1] (general chemical formula of Ketones). The chemical reactivity of the carbonyl group plays vital role in chemical reactions and is influenced considerably by steric effects. The greater electronegativity of O^- and high dipole moment value make Cyclohexanone polar. Scheme 1 illustrates this polarity. Further the presence of oxygen with its nonbonding electron pairs makes cyclohexanone H-bond acceptors. Thus a study on thermophysical properties data of binary liquid mixtures containing ketones has attracted considerable interest in the literature [5–9].

Literature survey reveals that Tsierkezos et al. [10] studied molecular interactions in cyclohexanone with methanol, ethanol, 1-propanol, 1-butanol, and 1-pentanol at 293.15 K and Sri Lakshmi et al. [11] studied molecular interactions in



Hindawi Publishing Corporation
Journal of Thermodynamics
Volume 2014, Article ID 487403, 13 pages
http://dx.doi.org/10.1155/2014/487403

Hindawi

Research Article

Thermoacoustic, Volumetric, and Viscometric Investigations in Binary Liquid System of Cyclohexanone with Benzyl Benzoate at $T = 308.15$, 313.15, and 318.15 K

Sk. Md Nayeem,[1] M. Kondaiah,[2] K. Sreekanth,[3] and D. Krishna Rao[4]

[1]*Department of Physics, KRK Govt. Degree College, Addanki 523 201, India*
[2]*Department of Physics, NM Govt. Degree College, Jogipet, Medak District, Telangana 502270, India*
[3]*Department of Physics, PBN College, Guntur District, Nidubrolu 522124, India*
[4]*Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar 522 510, India*

Correspondence should be addressed to D. Krishna Rao; krdhanekula@yahoo.co.in

Received 5 September 2014; Accepted 26 November 2014; Published 29 December 2014

Academic Editor: Ahmet Z. Sahin

Copyright © 2014 Sk. Md Nayeem et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

Ultrasonic velocities (u), densities (ρ), and viscosities (η) of binary liquid mixtures of cyclohexanone with benzyl benzoate, including pure liquids, over the entire composition range have been measured at 308.15 K, 313.15 K, and 318.15 K. Using the experimental results, parameters such as molar volume (V_m), isentropic compressibility (k_s), intermolecular free length (L_f), acoustic impedance (Z), internal pressure (π_i), enthalpy (H), Gibbs free energy of activation of viscous flow (G^{*E}), and excess/deviation properties of these including partial molar volumes ($\overline{V}_{m,1}$ and $\overline{V}_{m,2}$), excess partial molar volumes ($\overline{V}^E_{m,1}$ and $\overline{V}^E_{m,2}$), partial molar volume of the components at infinite dilution ($\overline{V}^{\infty}_{m,1}$, $\overline{V}^{\infty}_{m,2}$), and excess partial molar volume at infinite dilution ($\overline{V}^{E,\infty}_{m,1}$ and $\overline{V}^{E,\infty}_{m,2}$) have been computed. The observed negative values of V^E_m, Δk_s, L^E_f, and π^E_i and positive values of z^E, H^E, ΔG^{*E}, $\Delta\eta$, and Δu for all the liquid mixtures studied clearly indicate the presence of strong dipole-dipole-type interactions, fitting of smaller molecules into bigger molecules. Further theoretical values of sound velocity and viscosity in the mixtures have been evaluated using various theories and have been compared with experimental values to verify the applicability of such theories to the systems studied.

1. Introduction

Volumetric, viscometric, and ultrasonic investigations of liquid mixtures are of considerable importance in understanding the intermolecular interactions occurring among component molecules and they find application in several industrial and technological processes [1, 2]. The work on medicinally used chemical compounds requires the attention of the society in all aspects including ultrasonic behaviour. Benzyl benzoate is a carboxylate ester which is used in oily injections and as an insect repellent and as acaricide and pediculicide in veterinary hospitals. It is an effective and inexpensive topical treatment for human scabies. It is a polar ($\mu = 2.06$ D) molecule ($C^+{=}O^-$) with the structure shown in Figure 12. Behaviour of benzyl benzoate in many liquids such as aliphatic alkanes, aromatic alkanes, aliphatic alcohols, substituted benzenes, acetates, ketones, and DMSO (super solvent) has been thoroughly studied ultrasonically [3–6].

Ketone is an organic compound that contains a carbonyl group and two aliphatic or aromatic substituents containing the chemical formula $RCOR^1$. Here, R and R^1 may be same or different incorporated into a ring (alkyl, aryl, and heterocyclic radicals). Cyclohexanone is a ketone liquid. The chemical reactivity of the carbonyl group ($C^+{=}O^-$) plays important role in chemical reactions and is influenced considerably by steric effects. The greater electronegativity of O^- and high dipole moment make ketones polar ($\mu = 3.25$ D). The resonance structure shown in Figure 12 illustrates this polarity. Thus a study on thermophysical properties data of binary liquid mixtures has attracted considerable interest in the literature

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

The Journal of Chemical Thermodynamics
Volume 154, March 2021, 106330

A molecular interactions study between 1-butyl-3-methylimidazolium hexafluorophosphate ([Bmim][PF_6]) and N-methylpyrrolidone

Sowjanya Prathipati [a], Srinivasa Rao Vipparla [a, b], Srinivasa Reddy Munnangi [c], Md Nayeem Sk [d], Hari Babu Bollikolla [a]

Show more

+ Add to Mendeley Share Cite

https://doi.org/10.1016/j.jct.2020.106330

Get rights and content

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Author's Copy

GIF: Impact Factor 2012: 0.621
GIF: Impact Factor 2013: 0.723

E-ISSN NO: 2249-1929

Journal of Chemical, Biological and Physical Science

An International Peer Review E-3 Journal of Science

Section C : Physical Sciences

J. Chem. Bio. Phy. Sci. Sec. C, May 2014 - July 2014; Vol.4, No.3; 2401-2415.

Ultrasonic, Volumetric and Viscometric Study of Aqueous - Electrolyte Solutions

M. Kondaiah, K. Sreekanth, Sk.Md. Nayeem and D. Krishna Rao

*Corresponding author: D. Krishna Rao

Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar – 522 510, A.P., India

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Beebi et al., J Thermodyn Catal 2016, 7:4
DOI: 10.4172/2157-7544.1000177

Journal of Thermodynamics & Catalysis

Research Article OMICS International

Viscometric Study of Molecular Interactions in Dimethyl Carbonate +n-Alkoxyethanol Mixtures at Different Temperatures

SK Beebi[1,4], SKM Nayeem[2], GR Satyanarayana[3], A Venkateshwara Rao[1], D Bala[1] and C Rambabu[1]*

[1]Department of Chemistry, Acharya Nagarjuna University, Guntur, Andhra Pradesh, India
[2]Department of Physics, KRK Government Degree College, Addanki, Andhra Pradesh, India
[3]Department of Chemistry, Sir CR Reddy College, Eluru, Andhra Pradesh, India
[4]Department of Chemistry, YVNR Government Degree College, Kaikaluru, Andhra Pradesh, India

Abstract

The viscosities (η) and densities (ρ) have been measured for the binary mixtures of dimethyl carbonate (DMC) with 2-alkoxyethanols such as 2-methoxyethanol (MOE), 2-ethoxyethanols (EOE) and 2-butoxyethanols (BOE) over the entire range of mole fraction at T=(303.15, 308.15, 313.15, 318.15) K and at constant atmospheric pressure. The excess/deviation properties such as deviation in viscosity and excess Gibbs free energy of activation of viscous flow are calculated. Excess/deviation properties are correlated by the Redlich-Kister equation to obtain the binary coefficients and standard deviations. Further several semi empirical models such as Grunberg-Nissan, Katti-Chaudhri, Heric-Brewer and Hind et al. are used to correlate the viscosity of binary mixtures. The values of Δη, which refers to the deviation of the experimental values of the viscosity of the mixture from the mole fraction mixture law rules, are found to be negative for all the mixtures. The results are discussed in terms of molecular interactions due to physical, chemical and structural effects between the unlike molecules.

Keywords: Viscosity; Gibbs free energy; Redlich-Kister equation; Molecular interaction

Introduction

Viscosity and density data for binary liquids are important from practical and theoretical point of view. Experimental measurements of these properties of binary mixtures have gained much importance in many chemical industries and engineering disciplines [1]. Knowledge of the viscosity is very important in many chemical applications, such as mass and heat transfer operations, fluid flow, molecular structure and design involving chemical separations, developing separation methods like HPLC and capillary electrophoresis etc. Dimethyl carbonate (DMC) is considered to be a green solvent. It is a nontoxic substance and is widely used as a replacement for dimethyl sulphate, methyl halide, and phosgene in methylation and carbonylation reactions, because it is considered to be an "environmentally benign building block" [2]. Dialkyl carbonates have shown to be very useful in the lithium battery technology [3,4]. DMC has about 3 times the oxygen content as methyl tert-butyl ether (MTBE) and it is a strong contender to assist the refining industry. It does not phase separate in a water stream as some alcohols do, and it has both low toxicity and relatively quick biodegradability [5,6]. Glycol ethers are a group of solvents based on alkyl ethers of ethylene glycol or propylene glycol commonly used in paints and cleaners. Among cellosolves i.e., Alkoxyethanols viz. 2-methoxyethanol (MOE), 2-ethoxyethanol (EOE), 2-butoxyethanol (BOE) as oxygenated compounds are increasingly used as additives to gasoline due to their octane enhancing and pollution-reducing properties [7,8]. One of the interesting features of the chemicals that are selected in this study, are used as green solvents in gasoline industry.

In the present paper, we report viscosity, deviation in viscosity and excess Gibbs free energy of activation of viscous flow data for the binary mixtures of 2-methoxyethanol, 2-ethoxyethanol, 2-butoxyethanol with dimethyl carbonate at four different temperatures T=(303.15, 308.15, 308.15, 313.15) K. These Excess/deviation properties are correlated by the Redlich-Kister equation to obtain their binary coefficients and standard deviations. This work will also provide a test of various semi empirical relations like Grunberg-Nissan, Katti-Chaudhri, Heric-Brewer and Hind et al. to correlate viscosity of binary mixtures. Literature about binary liquid with one of the solvent as dimethyl carbonate is plenty [9-14]. A deep literature survey reveals that no significant work is available on the binary mixtures of dimethyl carbonate and 2-alkoxyethanols at a temperature range of (303.15-318.15) K.

Materials and Methods

DMC was obtained from Aldrich Chemical Co., stated purity 99 mol%. The chemicals 2-methoxyethanol, 2-ethoxyethanol and 2-butoxyethanol are obtained from SD Fine Chemicals Ltd., India, stated mass fraction purity>0.995 are used in this study. Before measurements, all the liquids were kept in dark bottles, dried over molecular sieves (Union Carbide, type 4A), and degassed it ultrasonically. All the chemicals were purified by method described in literature [15,16]. The chemicals after purification were 99.8% pure and their purity was ascertained by GLC and also by comparing experimental values of density and viscosity, at 303.15 K with those reported in the literature, as presented in Table 1.

The binary mixtures are prepared gravimetrically using an electronic balance (Shimadzu AY120) with an uncertainty of $\pm 1 \times 10^{-7}$ kg and stored in airtight bottles. The uncertainty on mole fraction is estimated to be 1×10^{-4}. It is ensured that the mixtures are properly mixed and the measurement of the required parameters was done within one day of preparation.

*Corresponding author: C Rambabu, Department of Chemistry, Acharya Nagarjuna University, Guntur-522 510, Andhra Pradesh, India, Tel: +919949839299; E-mail: cibpublications@gmail.com

Received October 14, 2016; Accepted October 27, 2016; Published November 07, 2016

Citation: Beebi SK, Nayeem SKM, Satyanarayana GR, Venkateshwara Rao A, Bala D, et al. (2016) Viscometric Study of Molecular Interactions in Dimethyl Carbonate +n-Alkoxyethanol Mixtures at Different Temperatures. J Thermodyn Catal 7: 177. doi: 10.4177/2160-7544.1000177

Copyright: © 2016 Beebi SK, et al. This is an open-access article distributed under the terms of the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

COMPUTATION OF (i)ACTIVITY COEFFICIENTS (ii) EXCESS CHEMICAL POTENTIAL (iii) EXCESS MOLAR ENTHALPY BY PRIGOGINE-FLORY-PATTERSON THEORY FOR BINARY LIQUID SYSTEM AT T=308.15K

Sk. Md Nayeem[a*], Imran Khan[b], Sk. Nyamathulla[c], D. Sampurna Rao[a], P. Indira[a], M. Srinivasa Reddy[d], J. Mythri[d], P. Nirmala Kumari[e]

[a] Department of Physics, KRK Govt. Degree College, Addanki 523201, A.P., India

[b] Department of Chemistry, College of Science, Sultan Qaboos University, PO Box 36, PC 123, Muscat, Oman

[c] Department of Physics, Govt. Degree College, Naidupet 524126, A.P., India

[d] Department of Chemistry, KRK Govt. Degree College, Addanki 523201, A.P., India

[e] Department of Mathematics, KRK Govt. Degree College, Addanki 523201, A.P., India

Abstract

For an adequate choice of binary mixture for the possible application, the knowledge of their interaction with each other is an essential feature for predicting the reactivity and selectivity. Using the density (ρ), viscosity (η) and ultrasonic speed (u), for the binary liquid mixtures of n-hexane with 1,4-dioxane at temperature T=308.15 K, we have evaluated activity coefficients and excess chemical potential using Morgules, Porter, Wilson and Van laar equation. The studied system shows deviation to the ideality indicating the presence of interaction in the binary system. Further, the negative sign of excess chemical potential of the studied binary mixture reveals the dominance of weaker interactions.

Keywords

Ultrasonic speed, density, viscosity, interactions, activity coefficients, excess chemical potentials, excess molar enthalpy, PFP theory.

* Corresponding Author:shaikmahammadnayeem@gmail.com
Phone: +91-9866374987

Introduction

In continuation of our earlier research [1-5], an attempt has been made to evaluate activity coefficients and excess chemical potentials from the physicochemical parameters i.e., ultrasonic speed, density and viscosity. The liquids under investigation *n*-hexane+1,4-dioxane have been chosen on the basis of their industrial applications. These applications have greatly motivated the need for widespread information on the thermodynamic, acoustic, and transport properties of these chemicals and their mixtures. It is well known fact that, ultrasonic speed and related thermodynamic parameters are helpful as well as needed for characterizing thermodynamic and physico-chemical aspects of binary liquid mixtures such as molecular association and dissociation. These physico-chemical analyses are used to handle the mixtures of hydrocarbons, alcohols, aldehydes, ketones etc. The measurement of ultrasonic speed enables us to perform the accurate measurement of some useful acoustic and thermodynamic parameters and their excess values. 1,4-dioxane (an ether) is a colourless liquid with a faint sweet odour similar to that of diethyl ether. It is designated as one of the super solvents and being used for a variety of practical applications in the laboratory. *n*-hexane are important series of homologous, nonpolar and organic solvents. They have often been used in the study of solute dynamics because of their physicochemical properties as a function of its chain length. These are commercially used as solvents, in paints, coatings, rubber cement, as power fuel and in gasoline. These studies find several significant applications in industries. In view of the importance of these liquids and experimental data of *n*-hexane+1,4-dioxane system at

Dept. of Computer Science, Govt. College for Women(A),Guntur ISBN 978-93-85132-12-4

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Proceedings of the International Seminar on Physics and Chemistry of Materials and Applications (ISPCMA-2017), SPMH Kalasala, Machilipatnam, A.P., India. 4th - 5th January, 2017. pp.108-111.

Investigation of Molecular Interaction in Binary System through Activity Coefficients and Application of Prigogine-Flory-Patterson Theory to Evaluate Excess Molar Enthalpy at T=308.15K

Sk. Md Nayeem[1], Imran Khan[2], D. Sampurna Rao[1], P. Indira[1], M. Srinivasa Reddy[3], P. Nirmala Kumari[4] and Sk. Beebi[5]

[1]Department of Physics, [3]Department of Chemistry, [4]Department of Mathematics
KRK Govt. Degree College, Addanki, A.P., India
[2]Department of Chemistry, College of Science, Sultan Qaboos University, PO Box 36, PC 123, Muscat, Oman
[5]Department of Chemistry, Govt. Degree College, Kaikaluru, A.P., India
Email: [1]shaikmahammadnayeem@gmail.com

ABSTRACT

For an adequate choice of binary mixture for the possible application, the knowledge of their interaction with each other is an essential feature for predicting the reactivity and selectivity. Using the density (ρ), and ultrasonic speed (u),for the binary liquid mixtures of ethyl acetate with benzyl benzoate (BB) at temperature T=308.15 K, we have evaluated activity coefficients using Morgules, Porter, Van laar equation and computed excess molar enthalpy by PFP theory. The studied activity coefficients show the presence of molecular interactions and PFP theory correctly predicted the sign of excess molar enthalpy.

Keywords— *Ultrasonic speed, density, interactions, activity coefficients, PFP theory, excess molar enthalpy.*

1. INTRODUCTION

In continuation of our earlier research [1-5], an attempt has been made to evaluate activity coefficients from the physicochemical parameters i.e., ultrasonic speed and density. Our previous work [6] reported physicochemical data of binary liquid mixtures of ethylacetate + benzylbenzoate at different temperatures *T= (308.15/313.15/318.15) K* and under atmospheric pressure. The liquids under investigation EA+BB have been chosen on the basis of their medicinal and industrial applications. These applications have greatly motivated the need for widespread information on the thermodynamic, acoustic, and transport properties of these chemicals and their mixtures. The work on medicinally used chemical compounds necessitates the attention of the society in all features including ultrasonic behaviour. It has an extensive application in chemical industries, food-flavour sectors and in the pharmaceuticals. It is a solvent used in a wide range of applications, including printing inks, varnishes and car care chemicals and in the production of enamels, plastics and rubber. Ethyl acetate is used in food industry as a synthetic flavouring and in the pharmaceutical industry as an extraction solvent in the production of pharmaceuticals. Benzyl benzoate (BB) is used in different ways: in oily injections, as an insect repellent and as acaricide and pediculicide in veterinary hospitals. For this investigation, experimental data of EA+BB system at *T=308.15 K* [6]has been taken and extended for computing activity coefficients so as to account for the interaction which exists between EA and BB molecules. Further, it is well known fact that the study of excess thermodynamic properties, such as excess molar enthalpy/ molar volume/ molar Gibbs energy, is extremely vital to comprehend molecular interaction in mixtures and to build up and to investigate the applicability of solution theories and statistical models. In this work, Prigogine–Flory– Patterson model (PFP) which contains only one adjustable parameter, is also applied at *T=308.15 K* and tested the applicability of such theory to the experimentally derived values of H_m^E.

2. ACTIVITY COEFFICIENTS

Phase equilibria are essential for chemical separation process design. The imperfectness of the liquid phase is accounted by liquid-phase activity coefficients by means of thermodynamic models. Experimental data are frequently unavailable over the range of conditions of interest; hence, the required data must be estimated using one of a variety of approaches. Further, the data of activity coefficients are expected for engineering design purposes. This made us to attempt evaluation of activity coefficients for the present binary system. Generally, the activity coefficient is a unit less parameter that measures the deviation from ideality in a mixture. In liquid phase,

ISBN: 978-93-82570-84-4

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

A NEW APPROACH TO INVESTIGATE MOLECULAR INTERACTIONS IN BINARY SYSTEM: AN INSIGHT FROM ACTIVITY COEFFICIENT AND EXCESS CHEMICAL POTENTIAL

Sk. Md Nayeem[a*], Imran Khan[b], Sk. Nyamathulla[c], D. Sampurna Rao[a], P. Indira[a], M. Srinivasa Reddy[d], GV Lokeswara Reddy[e]

[a] Department of Physics, KRK Govt. Degree College, Addanki 523201, A.P., India
[b] Department of Chemistry, College of Science, Sultan Qaboos University, PO Box 36, PC 123, Muscat, Oman
[c] Department of Physics, Govt. Degree College, Naidupet 524126, A.P., India
[d] Department of Chemistry, KRK Govt. Degree College, Addanki 523201, A.P., India
[e] Department of Physics, SCNR Govt. Degree College, Proddatur 516360, A.P., India
[*] Corresponding Author: shaikmahammadnayeem@gmail.com Phone: +91-9866374987

Abstract:

For an adequate choice of binary mixture for the possible application, the knowledge of their interaction with each other is an essential feature for predicting the reactivity and selectivity. Using the density (ρ), viscosity (η) and ultrasonic speed of sound (u),for the binary liquid mixtures of cyclohexanone with benzyl benzoate at temperature T=308.15 K, we have evaluated activity coefficients and excess chemical potential using Morgules, Porter, Wilson and Van laar equation. The studied system shows negative deviation to the ideality indicating a stronger interaction in the binary system. Further, the positive sign of chemical potential of the studied binary mixture reveals the dominance of strong interactions.

Keywords: Speed of sound, density, viscosity, interactions, activity coefficients, excess chemical potentials.

1. INTRODUCTION:

In continuation of our earlier research [1-5], an attempt has been made to evaluate activity coefficients and excess chemical potentials from the physicochemical parameters i.e., ultrasonic speed, density and viscosity. The liquids under investigation (CH+BB) have been chosen on the basis of their medicinal and industrial applications. These applications have greatly motivated the need for widespread information on the thermodynamic, acoustic, and transport properties of these chemicals and their mixtures. The work on medicinally used chemical compounds necessitates the attention of the society in all features including ultrasonic behaviour. Benzyl benzoate (BB) is used in different ways: in oily injections, as an insect repellent and as acaricide and pediculicide in veterinary hospitals. It is an effective and inexpensive topical treatment for human scabies. Cyclohexanone (CH) and its derivatives are used in different ways: in the synthesis of pharmaceuticals, dyes, herbicides, pesticides, plasticizers, and rubber chemicals. For this investigation, experimental data of (CH+BB) system at T=308.15K [6]has been taken and extended for computing activity coefficients and excess chemical potentials[7] so as to account for the type of interaction which exists between CH and BB molecules.

2. RESULTS AND DISCUSSIONS:

Activity coefficients:

Phase equilibria are essential for chemical separationprocess design. The imperfectness of the liquid phase is accounted by liquid-phase activity coefficients by means of thermodynamic models. Experimental data are frequently unavailableover the range of

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Aug 2014 – Oct. 2014, Vol. 4, No. 4; 3092-3108. E- ISSN: 2249 –1929

Journal of Chemical, Biological and Physical Sciences

An International Peer Review E-3 Journal of Sciences

*Available online at*www.jcbsc.org

Section A: Chemical Sciences

CODEN (USA): JCBPAT Research Article

Volumetric and viscometric study of aqueous ethylene glycol in butan-2-ol and propan-2-ol

Sk. Md Nayeem[a], M. Kondaiah[b], K. Sreekanth[c] and D. Krishna Rao[d]

[a] Department of Physics, KRK Govt. Degree College, Addanki, A.P., India.
[b] Department of Physics, NM Govt. Degree College, Jogipet, Medak Dt, A.P., India
[c] Department of Physics, PBN College, Nidubrolu, Guntur Dt, A.P., India
[d] Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar, A.P., India

Received: 24 July 2014; **Revised:** 18 September 2014 **Accepted:** 22 September 2014

Abstract: Densities, ρ, and viscosities, η of 10 m and 5 m aqueous ethylene glycol solution in propan-2-ol and butan-2-ol have been measured over the entire composition range at 308.15 K. From this experimental data, excess molar volume, V_m^E, excess Gibbs free energy of activation of viscous flow, ΔG^{*E} and deviation in viscosity, $\Delta\eta$ have been determined. Negative values of V_m^E, positive values of ΔG^{*E} and $\Delta\eta$ are observed over the entire composition range in the mixtures studied. The partial molar volumes and excess partial molar volumes of the components at infinite dilution, $\overline{V}_{m,1}^{\infty}$, $\overline{V}_{m,2}^{\infty}$, $\overline{V}_{m,1}^{E,\infty}$, $\overline{V}_{m,2}^{E,\infty}$ have been also calculated. The observed negative and positive values of excess and deviations attributed to the existence of strong interactions such as geometrical fitting of smaller molecules into the voids created by larger molecules in the liquid mixtures. The data for all the investigated solutions have been compared with the theoretically estimated values using empirical relations such as, Grunberg and Nissan, Hind *et al* and Katti and Chaudhari.

Keywords: Density, Viscosity, Excess/deviation properties, Redlich-Kister polynomial, Empirical values of viscosity.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

INTERNATIONAL JOURNAL OF PHARMACEUTICAL, CHEMICAL AND BIOLOGICAL SCIENCES

Available online at www.ijpcbs.com

Research Article

VOLUMETRIC AND VISCOMETRIC STUDY OF AQUEOUS SOLUTION OF ETHYLENE GLYCOL, PROPYLENE GLYCOL IN *ISO*-PROPANOL

M. Kondaiah[1], K. Sreekanth[2], Sk. Md. Nayeem[3] and D. Krishna Rao[4*]

[1]NM Govt. Degree College, Jogipet, Medak Dt, Andhra Pradesh, India.
[2]PBN College, Nidubrolu, Guntur Dt, Andhra Pradesh, India.
[3]Govt. Degree College, Addanki, Prakasam Dt, Andhra Pradesh, India.
[4]Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar – 522 510, Andhra Pradesh, India.

ABSTRACT

Densities, ρ and viscosities, η of 0.5 m, 1.0 m and 1.5 m aqueous ethylene glycol and propylene glycol solutions in *iso*-propanol have been measured over the entire composition range at 308.15 K. From this experimental data, deviation in viscosity, Δη, excess free volume, V_f^E, excess internal pressure, π_i^E, excess enthalpy, H^E and excess Gibbs free energy of activation of viscous flow, ΔG^{*E} have been determined. It has been observed that viscosity increases first and attained a maximum value thereafter decreases. Negative values of V_f^E and positive values of Δη, π_i^E, H^E, ΔG^{*E} are observed over the entire composition range in the mixtures studied. The observed negative and positive values of various excess and deviation parameters are attributed to the existence of strong interactions such as geometrical fitting of smaller molecules into the voids created by larger molecules in the liquid mixtures. The measured values of viscosity for all the investigated solutions have been compared with the theoretically estimated values using empirical relations such as, Grunberg, Hind and Frenkel.

Keywords: Density, Viscosity, Excess free volume, Redlich-Kister polynomial.

1. INTRODUCTION

Aqueous solutions play a vital role for many geological processes in various environments, such as geothermal and magmatic hydrothermal settings. Ultrasonic energy is used in medicine, engineering, agriculture, defence and industry. It is found to be useful in studying the chemical processes and in synthesis of chemical substances in chemical industries. Water and alcohol mixtures show unique maxima and minima in their thermodynamic and acoustic properties at low alcohol concentrations[1-4]. The formation of such maxima/minima in aqueous solutions of electrolytes[5] and in non-aqueous solutions[6,7] is also reported in literature.

Thermodynamic and transport studies of aqueous non electrolyte solutions of 0.5 m, 1.0 m and 1.5 m ethylene glycol/propylene glycol (non-electrolytes) in iso-propanol have been presented in this work. Masso Sakura[8] reported the partial molar volumes of ethylene glycol and water solutions at multi temperatures 15, 25, 35 and 45°C. Speeds of sound and viscosities in aqueous poly (ethylene glycol) solutions at 303.15 K and 308.15 K were presented by Pal and Wazir Singh[9]. Kanhekar *et al*[10] studied the thermodynamic properties in aqueous solution of glycine at different temperatures. Molecular interionic interaction studies of divalent transition metal sulphates in aqueous ethylene glycol at different temperatures were studied by Thirumaran and

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

ISSN: 0974-2115
www.jchps.com Journal of Chemical and Pharmaceutical Sciences

Experimental and Theoretical Investigations of Ultrasonic Speed in Binary Liquid Mixtures of Benzyl Benzoate with Isomers of Butanol at T=308.15K

Sk. Nyamathulla[1*], Sk.Md Nayeem[2]
[1]Department of Physics, Govt. Degree College, Naidupet-524126, A.P., India.
[2]Department of Physics, KRK Govt. Degree College, Addanki-523201, A.P., India.
*** Corresponding Author: nyamphy@gmail.com, Ph: +91-9885495781**

ABSTRACT

Ultrasonic speed is measured at 2MHz frequency in the binary mixtures of Benzyl Benzoate with n-butanol/sec-butanol/tert-butanol and semi empirical values of ultrasonic speed have been evaluated at 308.15 K using Nomoto's relation, Vandeal's relation, Parsania's Impedance relation, Rao's and Junjie's method. Semi empirical values of ultrasonic velocities are compared with the experimental values and the validity of the theories is checked by calculating the percentage deviation and standard deviations. A good agreement has been found between experimental and Parsania's Impedance ultrasonic velocity.

KEY WORDS: Ultrasonic speed, density, Semi empirical speed models.

1. INTRODUCTION

Measurement of ultrasonic speed gives the valuable information about the physicochemical behaviour of the liquid and liquid mixtures. Ultrasonic speeds, densities and derived thermodynamic and acoustical parameters are of considerable interest in understanding the intermolecular interactions in binary as well as ternary liquid mixtures. In the chemical industry knowledge of the thermodynamic properties of non-electrolyte solutions is essential in the design involving chemical separation, heat transfer, mass transfer and fluid flow. Ultrasonic studies can also be used to determine the extent of complexation and to calculate the formation constant values of charge transfer complexes. Measurement of ultrasonic speed has been adequately employed in understanding the nature of molecular interaction in pure liquid and liquid mixtures. The practical application of mixed solvents rather than single solvent in industrial and biological process has been recognized all over the world as they provide a wide choice of solutions with appropriate properties.

The present study deals with the thermodynamic study of mixed solvent system at 308.15 K temperature. The liquids under investigation have been chosen on the basis of their industrial applications. These applications have greatly stimulated the need for extensive information on the thermodynamic, acoustic and transport properties of these solvents and their mixtures.

Benzyl benzoate is a carboxylate ester, which is used as an insect repellent, a medicine for scabies and also used in oily injections. Behaviour of benzyl benzoate in many liquids such as aliphatic alkanes, aromatic alkenes, aliphatic alcohols, substituted benzenes, acetates, ketones and DMSO (super solvent) has been thoroughly studied ultrasonically.

Alcohols are self-associated organic liquids, used for the synthesis of other organic compounds. They are also widely used as coupling and dispersing agents in the chemical, pharmaceutical and household industries and as carrier and extraction solvents for natural Products. Branching of alkyl group attached to the hydroxyl group results in abnormal behaviour of alcohols. The interaction of alcohol [s] with organic liquids is interesting due to its acidic nature. The O-H bonds in alcohols are polar and allow the release of the hydrogen atom as proton (H+). The order of acidity in alcohols is: 1°-alcohol> 2°- alcohol > 3°-alcohol. This order is due to +I effect.

In continuation of our earlier work, we report the ultrasonic speed evaluated using Nomoto's relation, Impedance relation, Ideal mixture relation and Junjie's method for the binary mixtures of Benzyl benzoate with n-butanol/sec-butanol/tert-butanol. Further, the best suitable theory for the given molecular system under study is also picked out by calculating the percentage deviation and standard error.

2. EXPERIMENTAL DETAILS

High purity Analytical Reagent (AR) grade samples of Benzyl benzoate (BB) (sd fine chemicals), n-butanol (Fluka), sec-butanol procured from Merck and tert-butanol procured from Sigma Aldrich were used. Before measurements all the liquids were carefully dried over 0.4 nm molecular sieves and stored in dark bottles. These samples were further purified by standard methods. The solutions of binary mixtures BB with AP, CH and 3P have been prepared in the specially designed glass bottles with air tight stoppers and adequate precautions have been taken to minimize evaporation losses. Before measurements all the liquids were carefully dried over 0.4 nm molecular sieves and stored in dark bottles. These samples were distilled just before use. The purity of these liquids was ascertained by Gas Chromatography (HP 8610) using a FID detector and the analysis indicated mole percent purities > 99.5 %. The weighing of solutions has been made using a METTLER TOLEDO (Switzerland make) ABB5-S/FACT digital balance with an accuracy of ±0.01 mg. The uncertainty in the mole fraction is 10-4. The ultrasonic speed (u) of pure liquids and liquid mixtures have been measured using an ultrasonic interferometer (Mittal type,

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

ISSN: 0974-2115
www.jchps.com Journal of Chemical and Pharmaceutical Sciences

Experimental and theoretical investigations of ultrasonic speed in binary liquid mixtures of ascabin with isomers of butanol at T=313.15K

Nyamathullaa Sk[1*], Nayeemb Md[2]
[1]Department of Physics, Govt. Degree College, Naidupet-524126, A.P., India.
[2]Department of Physics, KRK Govt. Degree College, Addanki-523201, A.P., India
***Corresponding author: E-Mail: nyamphy@gmail.com**

ABSTRACT

Ultrasonic speed is measured at 2MHz frequency in the binary mixtures of ascabin with n-butanol/sec-butanol/tert-butanol and semi empirical values of acoustic speed have been evaluated at 313.15 K using Nomoto's relation, Vandeal's relation, Parsania's Impedance relation, Rao's and Junjie's method. Semi empirical values of acoustic speeds are compared with the experimental values and the validity of the theories is checked by calculating the percentage deviation. A good agreement has been found between experimental and Nomoto's ultrasonic speed.

KEY WORDS: Ultrasonic speed, density, semi empirical speed models.

1. INTRODUCTION

Measurement of acoustic speed gives the precious information about the physicochemical behaviour of the liquid and binary liquid mixtures. Ultrasonic speeds, densities and derived thermodynamic and acoustical parameters are of considerable interest in establishing molecular interactions in binary and ternary liquid mixtures. In the chemical industry knowledge of the thermodynamic properties of non-electrolyte solutions is essential in the design involving, heat shift, chemical partition, mass shift and fluid flow. Acoustic studies can also be used to find out the degree of complexation and to calculate the formation constant values of charge shift complex. Measurement of ultrasonic speed has been sufficiently employed in establishing the type of molecular interaction in pure liquid and liquid mixtures. The useful application of mixed solvents rather than single solvent in industrial and biological process has been accepted all around the world as they give a wide choice of solutions with relevant properties.

The present study deals with the thermodynamic study of mixed liquid system at 313.15 K temperature. The liquids under exploration have been chosen on the basis of wide applications and industrial importance. These applications have intensely stimulated the need for broad and depth information on the thermodynamic, acoustic, transport properties of these solvents and their mixtures.

Ascabin is a carboxylate ester, which is used as pest repellent, drug for skin related diseases and oily injection. Behaviour of ascabin in various liquids such as aliphatic alkanes, aromatic alkenes, aliphatic alcohols, substituted benzenes, acetates, ketones and DMSO (super solvent) has been systematically studied acoustically.

We know that alkanols are self- connected organic liquids, used for the production of several organic compounds. They are also widely used as coupling and dispersing agent in the pharmaceutical, chemical and domestic industry and as a transporter and extraction of solvents for natural products. Branching of CH3 group attached to the -OH group results in anomalous behaviour of alcohols. The action of alkanol [s] with organic liquids is remarkable due to its acidic property. The O-H bonds in alkanols are polar and allow the liberation of the H atom as proton (H+). The order of acidity in alcohols is: 1°-alcohol> 2°- alcohol > 3°-alcohol. This order is due to +I effect.

As an extension of our earlier work, we report here the acoustic speed evaluated using Nomoto's relation, Impedance relation, Ideal mixture relation and Junjie's method for the binary mixtures of Ascabin with n-butanol/sec-butanol/tert-butanol. Moreover, the best suitable theory for the given molecular system under study is also picked out by deriving the percentage deviation.

2. EXPERIMENTAL DETAILS

High purity Analytical Reagent (AR) grade samples of Ascabin (BB) (sd fine chemicals), n-butanol (Fluka), sec-butanol procured from Merck and tert-butanol procured from Sigma Aldrich were used. Before the experiment, all the chemicals were cautiously dried over 0.4 nm molecular sieves and stored in dark bottles. These chemicals were further purified by standard methods.

The solutions of binary mixtures BB with alkanols have been prepared in the specially designed glass bottles with air tight stoppers and suitable measures have been taken to minimize evaporation losses. All the binary liquids were carefully dried over 0.4 nm molecular sieves further and stored in clear dark bottles well before the measurements. These binaries were distilled just before use.

The purity of these binaries was measured by Gas Chromatography (HP 8610) using a FID detector and the analysis indicated mole percent purities > 99.5 %. The weighing of binaries has been made with a METTLER TOLEDO (Switzerland make) ABB5-S/FACT digital balance with an accuracy of ±10-2 mg. The uncertainty in the mole fraction is 10-4.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

National Conference on Advanced Functional Materials and Computer Applications in Materials Technology (CAMCAT-2014)
Indian Journal of Research in Pharmacy and Biotechnology ISSN: 2320-3471 (Online); 2321-5674 (Print)

Study of some thermodynamic and acoustic properties in the solutions of acrylamide with equimolar mixture of ethanol and isopropylalcohol/isobutyl alcohol/isoamylalcohol

K. Sreekanth[1], D. Sravana Kumar[2], M. Kondaiah[3], Sk. Md. Nayeem[4], Sk. Akram[1], D. Krishna Rao[5]*
1. Department of Physics, PBN College, Nidubrolu, Guntur Dt, A.P., India.
2. Department of Physics, Dr.V.S.Krishna Govt. Degree College, Visakhapatnam, 530 013, Andhra Pradesh, India.
3. Department of Physics, NM Govt. Degree College, Jogipet, Medak Dt, Telangana, India.
4. Department of Physics, KRK Govt. Degree College, Addanki-523 201, A.P., India.
5. Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar- 522510,Andhra Pradesh, India
***Corresponding author: Email: krdhanekula@yahoo.co.in**

ABSTRACT

Ultrasonic speeds (u), densities (ρ) and viscosities (η) of the solutions of acrylamide as solute with equimolar mixture of ethanol and isopropyl alcohol(EIP)/isobutyl alcohol(EIB)/isoamyl alcohol(EIA) as solvent including those of pure liquids have been measured at 308.15 K. From the experimental data of u, ρ and η the isentropic compressibility (k_s), intermolecular freelength (L_f), acoustic impedance (Z), molar volume (V_m), internal pressure (π_i), enthalpy (H), viscous relaxation time (τ) and relative association (R_A) have been calculated. The variation of these parameters with the molality of acrylamide is helpful to understand the nature and extent of molecular interactions between unlike molecules in the solutions. Further, the experimental results have been analyzed on the basis of dipole – dipole interactions, strong interactions such as -C = O……H-O- hydrogen bonding.

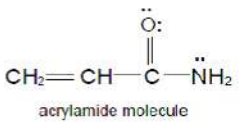
Key Words: acrylamide, isentropic compressibility, internal pressure, molecular interactions, dipole-dipole interactions, hydrogen bonding.

1. INTRODUCTION

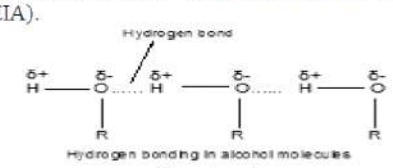
The ultrasonic speed has been adequately employed in understanding the nature of molecular systems and physicochemical properties in liquid mixtures (Iloukhani et al, 1995). The non linear behavior of ultrasonic speed, compressibility and other acoustical, thermo dynamical parameters of solute-solvent solutions with concentration of solute is attributed to the difference in size of the molecules and the strength of interactions. For the qualitative estimation of the molecular interactions in solutions, the ultrasonic velocity approach was first studied by Lagemann and Dunbar (1945).

Mixed solvents find more practical applications in chemical, industrial and biological processes, because they provide a wide range of desired properties compared to their pure solvents. The studies of physicochemical properties of amide+secondary alkanol solutions are of very interesting because the amide is convenient system for investigating the peptide and protein solvent interactions. Acrylamide (A) an organic solid compound is used to synthesize polyacrylamides which find many uses as water soluble thickeners, waste water treatment, gel electrophoresis, paper making, reprocessing, manufacture of dyes and the manufacture of other monomers. The use of alcohols in preparing a number of compounds like aldehydes, ketones, acids, alkenes, alkanes, alynes, halides , etc., are well known. Acrylamide molecules are highly polar in nature (μ = 3.44 D) and are strongly associated through three hydrogen bond donors (3H – atoms) and three acceptors (two lone pairs of electrons at oxygen and one on nitrogen atom) as shown in structure 1. Secondary alkanol molecules are polar and self associated through hydrogen bonding of their hydroxyl groups as shown in structure 2. The components of these solutions have both proton donating/accepting ability, significant interaction through hydrogen bonding between unlike molecules.

Research survey reveals that very little quantity of work was reported in the solutions of acrylamide (Sravan Kumar, 1995; Chennappan and Sankar, 2004). To the best of our knowledge, there has been no work on acoustic and thermodynamic parameters reported in the solutions of acrylamide (A) as solute with equimolar mixture of ethanol and isopropylalcohol(EIP) /isobutylalcohol(EIB)/isoamylalcohol(EIA).



Structure 1



Structure 2

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

International Journal of Pharma Research & Review, Feb 2014; 3(2):65-78 ISSN: 2278-6074

Research Article

Ultrasonic Investigations of Molecular Interaction in Binary Mixtures of Benzyl Benzoate with Isomers of Butanol

Sk Md Nayeem[a] and *D.Krishna Rao[b]

a. Department of Physics, KRK Govt. Degree College, Addanki-523 201, A.P., India.

b. Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar – 522 510, A.P., India

ABSTRACT

The density and speed of sound have been measured for the systems (Benzyl Benzoate + *n*-butanol, *sec*-butanol, *tert*-butanol) at different molefraction and at different temperatures 308.15K, 313.15K respectively. From these experimental data the excess/ deviation acoustic parameters such as deviation in isentropic compressibility, excess intermolecular free length, excess acoustic impedance and deviation in ultrasonic velocity have been calculated for the binary systems at 308.15 K and 313.15 K temperatures. The calculated excess / deviation functions have been fitted to Redlich-Kister polynomial using multi parametric non-linear regression analysis to estimate the coefficients and standard errors. The variation of these properties with composition and temperature of the binary mixtures have been studied in terms of molecular interactions between unlike molecules of the mixtures. Further, the results are supported by FTIR spectra.

Keywords: Benzyl Benzoate, *n*-butanol, *sec*-butanol, *tert*-butanol, ultrasonic velocity, density, excess / deviation parameters, Redlich-Kister polynomial, intermolecular interaction, FTIR spectra.

Received 25 Sept 2013 Received in revised form 11 Oct 2013 Accepted 14 Oct 2013

***Address for correspondence:**
Prof. D.Krishna Rao
Department of Physics, Acharya Nagarjuna University, Nagarjuna Nagar – 522510, India. Email : krdhanekula @ yahoo.co.in

INTRODUCTION

The work on medicinally used chemical compounds requires the attention of the society in all aspects including ultrasonic behavior. Practically, ultrasonic studies are of immense use to study the molecular interactions when these compounds are in binary mixture form with some other liquids - protic /aprotic /polar /non-polar *etc*. Benzyl Benzoate (bb) is a carboxylate ester, which is used as an insect repellent, a medicine for scabies and also used in oily injections. Behavior of benzyl benzoate in many liquids such as aliphatic alkanes, aromatic alkenes, aliphatic alcohols, substituted benzenes, acetates, ketones and DMSO (super solvent) [1-4] has been thoroughly studied ultrasonically.

Alcohols are self-associated organic liquids, used for the synthesis of other organic compounds. They are also widely used as coupling and dispersing agents in the chemical, pharmaceutical and household industries and as carrier and extraction solvents for natural Products. Branching of alkyl group attached to the hydroxyl group results in abnormal behavior of alcohols. The interaction of alcohol [s] with organic liquids is interesting due to its acidic nature. The O-H bonds in alcohols are polar and allow the release of the hydrogen atom as proton (H+). The order of acidity in alcohols is: 1°-alcohol> 2°- alcohol > 3°-alcohol. This order is due to +I effect [5].

While the interacting ability of alcohols is well established, no such opinion is suggested from literature with regards to Benzyl Benzoate. Keeping this in view; three binary liquid mixtures *n*-butanol, *sec*-butaol and *tert*-butaol with Benzyl Benzoate were selected to study their molecular interactions through their acoustical behavior at two temperatures

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

WOODHEAD PUBLISHING SERIES IN COMPOSITES SCIENCE AND ENGINEERING

Cellulose-Reinforced Nanofibre Composites

Production, Properties and Applications

Edited by Mohammad Jawaid, Sami Boufi, and Abdul Khalil H.P.S.

WP
WOODHEAD PUBLISHING

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Woodhead Publishing is an imprint of Elsevier
The Officers' Mess Business Centre, Royston Road, Duxford, CB22 4QH, United Kingdom
50 Hampshire Street, 5th Floor, Cambridge, MA 02139, United States
The Boulevard, Langford Lane, Kidlington, OX5 1GB, United Kingdom

Copyright © 2017 Elsevier Ltd. All rights reserved.

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopying, recording, or any information storage and retrieval system, without permission in writing from the publisher. Details on how to seek permission, further information about the Publisher's permissions policies and our arrangements with organizations such as the Copyright Clearance Center and the Copyright Licensing Agency, can be found at our website: www.elsevier.com/permissions.

This book and the individual contributions contained in it are protected under copyright by the Publisher (other than as may be noted herein).

Notices

Knowledge and best practice in this field are constantly changing. As new research and experience broaden our understanding, changes in research methods, professional practices, or medical treatment may become necessary.

Practitioners and researchers must always rely on their own experience and knowledge in evaluating and using any information, methods, compounds, or experiments described herein. In using such information or methods they should be mindful of their own safety and the safety of others, including parties for whom they have a professional responsibility.

To the fullest extent of the law, neither the Publisher nor the authors, contributors, or editors, assume any liability for any injury and/or damage to persons or property as a matter of products liability, negligence or otherwise, or from any use or operation of any methods, products, instructions, or ideas contained in the material herein.

British Library Cataloguing-in-Publication Data
A catalogue record for this book is available from the British Library

Library of Congress Cataloging-in-Publication Data
A catalog record for this book is available from the Library of Congress

ISBN: 978-0-08-100957-4 (print)
ISBN: 978-0-08-100965-9 (online)

For information on all Woodhead Publishing publications
visit our website at https://www.elsevier.com/books-and-journals

Publisher: Mathew Deans
Acquisition Editor: Gwen Jones
Editorial Project Manager: Edward Payne
Production Project Manager: Debasish Ghosh
Cover Designer: Greg Harris

Typeset by MPS Limited, Chennai, India

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Mohamed M. Khattab Ryerson University, Toronto, ON, Canada

Jalel Labidi University of the Basque Country UPV/EHU, Donostia, Spain

Norhene Mahfoudhi University of Sfax, Sfax, Tunisia

M.M. Marliana University of Technology, Malaysia, Johor Bahru, Malaysia

Sk. Md Nayeem KRK Government Degree College, Addanki, Andhra Pradesh, India

M.K. Mohamad Haafiz University of Science, Malaysia, Penang, Malaysia

Dibyendu Mondal University of Aveiro, Aveiro, Portugal

Robert J. Moon USDA-Forest Service, Madison, WI, United States; Georgia Institute of Technology, Atlanta, GA, United States; Purdue University, West Lafayette, IN, United States

Pere Mutjé University of Girona, Girona, Spain

Mohammed Nasir Universiti Science Malaysia, Penang, Malaysia

Mohammad R. Nurul Fazita University of Science, Malaysia, Penang, Malaysia

Abdulwahab F. Owolabi Federal Institute of Industrial Research Oshodi, Lagos, Nigeria

Md T. Paridah Universiti Putra Malaysia, Selangor, Malaysia

Kalyani Prusty Veer Surendra Sai University of Technology, Sambalpur, Odisha, India

Abou el Kacem Qaiss Moroccan Foundation for Advanced Science, Innovation and Research, Rabat, Morocco

Mahmoud Rababah The Hashemite University, Zarqa, Jordan

Medyan Riza Syiah Kuala University, Banda Aceh, Indonesia

Eduardo Robles University of West Hungary, Sopron, Hungary; University of the Basque Country UPV/EHU, Donostia, Spain

Enih Rosamah Mulawarman University, Samarinda, East Kalimantan, Indonesia

Naheed Saba Universiti Putra Malaysia, Selangor, Malaysia

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Biomass nanofibrillar cellulose in nanocomposites

13

Mohd A. Usmani[1,6], Imran Khan[2], Sk. Md Nayeem[3], Dibyendu Mondal[4], Aamir H. Bhat[5], Imran Ahmed[1] and Asharul Haque[2]
[1]Eritrea Institute of Technology, Asmara, Eritrea [2]Sultan Qaboos University, Muscat, Oman [3]KRK Government Degree College, Addanki, Andhra Pradesh, India [4]University of Aveiro, Aveiro, Portugal [5]Universiti Teknologi PETRONAS, Perak, Malaysia [6]Gandhi Faiz-E-Aam College, Shahjahanpur, Uttar Pradesh, India

13.1 Introduction

Cellulose is a natural homopolymer present in the cell walls of many plants. Industrially it has been utilized mostly for manufacture of cardboard and paper but in recent times it has also gained attention as a major resource of biofuel production. Lignocellulosic materials in forests are considered the primary source of cellulose on earth, having wood as the chief source. The rest of the materials having cellulose comprise agriculture residues, grasses, water plants, and other plant matters. Along with cellulose, they also possess hemicelluloses and lignin. Industrial production of cellulose depends mostly on harvested resources like wood or on naturally clean resources, for instance, cotton. The structure and orientation of cellulose in the cubicle walls of straw have been described [1]. The field of nanocellulose fibers as a loading phase in nanocomposites was initiated two decades ago [2]. Since then, a vast amount of literature has been created on nanocellulose fibers, and it is gradually becoming a more relevant issue. Crystalline rod-like nanoparticles have been termed "whiskers," while the designation "nanofibrils" refers to elongated elastic nanoparticles having discontinuous crystalline and amorphous filaments.

Cellulose fibers possess an exclusive hierarchy structure developed biologically. They contain nanofiber bunches of diameter 2–20 nm, and of length higher than only a few micrometers. In effect, the main reason to employ nanocellulose fibers in composite materials is to potentially develop greater hardness of the cellulose crystal for loading. This can be completed by reducing the hierarchical structure of the plant into single nanofibers of high crystallinity, thus bringing down the quantity of amorphous material. The hierarchical fibers make them able to do this; therefore, because of their aspect ratio (length/diameter) loading abilities are highly favorable for composite materials. The purpose of this chapter is to present current research in the field of nanocellulose fibrils and their application through illustrations. Also, it has been investigated that cellulose as a naturally manufactured product relates to the polymers that showed an extraordinary future ability for elementary facts and for large-scale synthesis in numerous applications [3].

Cellulose-Reinforced Nanofibre Composites. DOI: http://dx.doi.org/10.1016/B978-0-08-100957-4.00013-9
Copyright © 2017 Elsevier Ltd. All rights reserved.

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

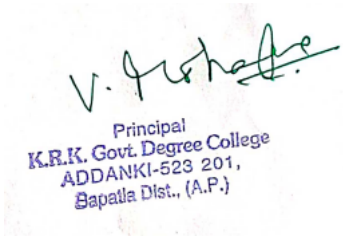
Edited by

Mohammad Jawaid
Universiti Putra Malaysia, Selangor, Malaysia

Sami Boufi
University of Sfax, Sfax, Tunisia

Abdul Khalil H.P.S.
University of Science, Malaysia, Penang, Malaysia

WP
WOODHEAD
PUBLISHING
An imprint of Elsevier



Trainings

CENTRE FOR CONTINUING EDUCATION
INDIAN INSTITUTE OF TECHNOLOGY MADRAS

Certificate of Completion

This certificate is awarded to

Shaik Mahammad Nayeem

for successfully completing the course

Computer-Aided Drug Design For SARS-CoV-2

from April 8th to April 9th 2022

Prof. Andrew Thangaraj
Coordinator,
NPTEL, IIT Madras

Devendra Jalihal

Prof. Devendra Jalihal
Chairman
Centre for Continuing Education, IIT Madras

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Prof. Niranjan Kumar
Department of Hindi, Faculty of Arts,
University of Delhi, Delhi- 110007
Ex Lecturer, University of California, **USA**
Ex Lecturer, Arizona State University, **USA**
Ex Lecturer, University of Michigan, **USA**
Ex Reader/ Asso. Professor, AMU, Aligarh

Dean of Planning
University of Delhi
Off.: 011-27662985
Email: nkumar@hindi.du.ac.in
dean_planning@du.ac.in
Twitter: @Niranjankindia

University of Delhi

Nodal Officer for Evaluation of **SWAYAM Engineering Courses' Translation, Ministry of Education, Government of India**

Dated: June 22, 2022

To Whomsoever it may concern

This is to certify that **Dr. Shaik Mahammad Nayeem** participated as a subject expert in the evaluation work for the translation of first-year engineering SWAYAM courses in regional languages. The project is undertaken by the University of Delhi directly under the Ministry of Education, Government of India. The project aims to recognize experts' opinions and evaluate the speech-to-speech machines (translation, subtitling, Dubbing/voice-over) to ensure the good quality of content in English and other regional languages.

Dr. Shaik Mahammad Nayeem has evaluated the video lectures of the following courses:

Course name:	**Introductory Quantum Mechanics**
Language:	**Telugu**
No. of lectures evaluated:	**55**

Thank you for all the work you have done and for being a part of the expert panel. We appreciate all the time and effort you provided.

Yours sincerely,

Prof. Niranjan Kumar
Dean (Planning)
Nodal Officer & Chairman for Swayam Evaluation Courses
University of Delhi

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Prof. Niranjan Kumar
Department of Hindi, Faculty of Arts,
University of Delhi, Delhi- 110007
Ex Lecturer, University of California, **USA**
Ex Lecturer, Arizona State University, **USA**
Ex Lecturer, University of Michigan, **USA**
Ex Reader/ Asso. Professor, AMU, Aligarh

Dean of Planning
University of Delhi
Off.: 011-27662985
Email: nkumar@hindi.du.ac.in
dean_planning@du.ac.in
Twitter: @Niranjankindia

University of Delhi

Nodal Officer for Evaluation of SWAYAM Engineering Courses' Translation, Ministry of Education, Government of India

---

Dated: June 22, 2022

To Whomsoever it may concern

This is to certify that **Dr. Shaik Mahammad Nayeem** participated as a subject expert in the evaluation work for the translation of first-year engineering SWAYAM courses in regional languages. The project is undertaken by the University of Delhi directly under the Ministry of Education, Government of India. The project aims to recognize experts' opinions and evaluate the speech-to-speech machines (translation, subtitling, Dubbing/voice-over) to ensure the good quality of content in English and other regional languages.

Dr. Shaik Mahammad Nayeem has evaluated the video lectures of the following courses:

Course name:	**Quantum Mechanics -I**
Language:	**Telugu**
No. of lectures evaluated:	**71**

Thank you for all the work you have done and for being a part of the expert panel. We appreciate all the time and effort you provided.

Yours sincerely,

Prof. Niranjan Kumar
Dean (Planning)
Nodal Officer & Chairman for Swayam Evaluation Courses
University of Delhi

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

Prof. Niranjan Kumar
Department of Hindi, Faculty of Arts,
University of Delhi, Delhi- 110007
Ex Lecturer, University of California, **USA**
Ex Lecturer, Arizona State University, **USA**
Ex Lecturer, University of Michigan, **USA**
Ex Reader/ Asso. Professor, AMU, Aligarh

Dean of Planning
University of Delhi
Off.: 011-27662985
Email: nkumar@hindi.du.ac.in
dean_planning@du.ac.in
Twitter: @Niranjankindia

University of Delhi

Nodal Officer for Evaluation of SWAYAM Engineering Courses' Translation, Ministry of Education, Government of India

---

Dated: June 22, 2022

To Whomsoever it may concern

This is to certify that **Shaik Mahammad Nayeem** participated as a subject expert in the evaluation work for the translation of first-year engineering SWAYAM courses in regional languages. The project is undertaken by the University of Delhi directly under the Ministry of Education, Government of India. The project aims to recognize experts' opinions and evaluate the speech-to-speech machines (translation, subtitling, Dubbing/voice-over) to ensure the good quality of content in English and other regional languages.

Shaik Mahammad Nayeem has evaluated the video lectures of the following courses:

Course name: **Waves and Oscillations**

Language: **Telugu**

No. of lectures evaluated: **58**

Thank you for all the work you have done and for being a part of the expert panel. We appreciate all the time and effort you provided.

Yours sincerely,

Prof. Niranjan Kumar
Dean (Planning)
Nodal Officer & Chairman for Swayam Evaluation Courses
University of Delhi

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

AD Scientific Index

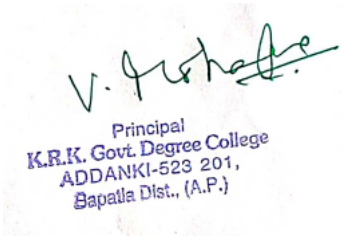
Rankings for Scientist

University, Subject, Country, Region, World

World Scientist and University Rankings 2021

K R K Government Degree College Addanki

SK. Md Nayeem

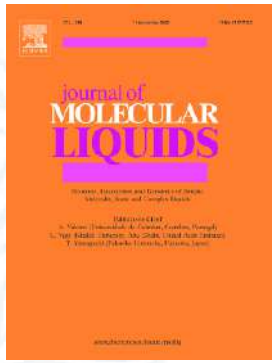


	Scores	In K R K Government Degree College Addanki (2)	In India (30184)	In Asia (167693)	World (749753)
		Rankings			
Total H	10	#1	#20226	#116065	#518354
Last 5 year H	9	#1	#17663	#102507	#426608
Last 5 year H / total H	0.900				
Total i10	10	#1	#22246	#124314	#546240
Last 5 years i10	8	#1	#18691	#109967	#460705
Last 5 years i10 / Total i10	0.800				
Total Citation	909	#1	#27549	#154852	#719299
Last 5 years Citation	718	#1	#23433	#142731	#649803
Last 5 years Citation / Total Citation	0.790				
Natural Sciences *		#1 (1) *	#5157 (6256) *	#22019 (25904) *	#88541 (103108) *
Physics *		#1 (1) *	#1610 (1903) *	#6581 (7498) *	#24809 (27528) *

www.adscientificindex.com

Date : 03.02.2022 * Source and Methodology: https://www.adscientificindex.com/scientist.php?id=2004927

ELSEVIER



Journal of Molecular Liquids

Certificate of Reviewing

Awarded since June 2020 (2 reviews)
presented to

SK. MD NAYEEM

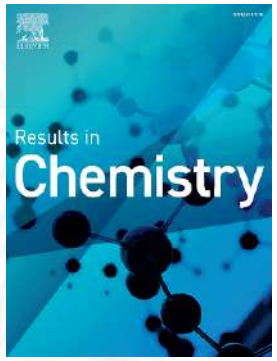
in recognition of the review contributed to the journal

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

The Editors of Journal of Molecular Liquids

Elsevier Reviewer RECOGNITION

ELSEVIER



Results in Chemistry

Certificate of Reviewing

Awarded since March 2020 (1 review)
presented to

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

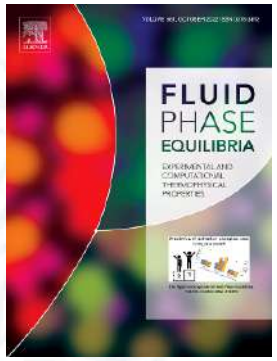
SK. MD NAYEEM

in recognition of the review contributed to the journal

The Editors of Results in Chemistry

Elsevier Reviewer RECOGNITION

ELSEVIER



Fluid Phase Equilibria

Certificate of Reviewing

Awarded since June 2021 (3 reviews)
presented to

Principal
K.R.K. Govt. Degree College
ADDANKI-523 201,
Bapatla Dist., (A.P.)

SK. MD NAYEEM

in recognition of the review contributed to the journal

The Editors of Fluid Phase Equilibria

Elsevier Reviewer RECOGNITION